SAND2022-6636R

Produced Water-Economic, Socio, Environmental Simulation Model (PW-ESEim) Model: Proof-of-Concept for Southeastern New Mexico

Vincent Tidwell, Thushara Gunda and Mariah Caballero: Sandia National Laboratories
Pei Xu and Xuesong Xu: New Mexico State University
Rich Bernknopf and Craig Broadbent: University of New Mexico
Len Malczynski and Jake Jacobson: Mindseye Consulting

May 2022

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

ABSTRACT

A proof-of-concept tool, the Produced Water-Economic, Socio, Environmental Simulation model (PW-ESESim), was developed to support ease of analysis. The tool was designed to facilitate head-to-head comparison of alternative produced water source, treatment, and reuse water management strategies. A graphical user interface (GUI) guides the user through the selection and design of alternative produced water treatment and reuse strategies and the associated health and safety risk and economic benefits. At the highest conceptual level, alternative water strategies include the selection of a source water (locally or regionally available produced water), treatment strategy (pre-treatment, physical, chemical, biological, desalination, and post-treatment processes) and product water purpose (e.g., irrigation, industrial processing, environmental). After selection of these details, the PW-ESESim output a number of key economic, societal, environmental, public/ecological health and safety metrics to support user decision-making; specific examples include, cost of treatment, improvements in freshwater availability, human and ecologic health impacts and growth in local jobs and the economy. Through the simulation of different produced water treatment and management strategies, tradeoffs are identified and used to inform fit-for-purpose produced water treatment and reuse management decisions. While the tool was initially designed using Southeastern New Mexico (Permian Basin) as a case study, the general design of the PW-ESESim model can be extended to support other oil and gas regions of the U.S.

ACKNOWLEDGEMENTS

This work was funded through the US Department of Energy's Office of Fossil Energy and Carbon Management. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

CONTENTS

LIST OF FIGURES

LIST OF TABLES

ACRONYMS AND DEFINITIONS

Abbreviation	Definition
ADRPOT	Acute Dose Rate
AT	Averaging Time
BW	Body Weight
cfs	cubic feet per second
COCs	constituents of concern
EPA	Environmental Protection Agency
ED	Exposure Duration
ESE	deleterious economic, societal, and environmental
ESG	environmental, social, and governance ESG
GUI	graphical user interface
GWPC	Groundwater Protection Council
ICMP	Industrial/Commercial/Mining/Power
LADCPOT	Lifetime Average Daily Concentration
LADDPOT	Lifetime Average Daily Dose
MOO	multi-objective optimization
NMOCD	NM Oil Conservation Division
NMPWRC	New Mexico Produced Water Research Consortium
NPDES	National Pollutant Discharge Elimination System
O&M	operation and maintenance
PW-ESESim	Produced Water-Economic, Socio, Environmental Simulation model
SAR	sodium absorption ratio
SD	System Dynamics
SDWA	Safe Drinking Water Act
TDS	total dissolved solids
WaDOH	Washington State Department of Health's

1. INTRODUCTION

1.1. Background

The oil and gas industry consumes and produces water. In 2012 the water used for oil and gas extraction was estimated at ~0.95 trillion gallons (Bauer et al. 2014) while produced water volumes were estimated at ~0.9 trillion gallons (Veil 2015). Rapid growth in the industry has led to both increased demand on freshwater as well as increased volumes of produced water that requires disposal or treatment for reuse. Treating produced water for beneficial reuse both inside and outside the oil and gas sector has become an attractive option; however, reuse outside the oil and gas sector is challenging because of poorly understood risks on public and environmental health and safety for fit-for-purpose treated water discharges; complexity in selecting appropriate treatment technologies and performance criteria; and highly variable wastewater quality and quantity. Ultimately, the means by which these waters are managed has the potential for both beneficial and deleterious economic, societal, and environmental (ESE) consequences (Dolan et al. 2018; O'Rourke and Connolly 2003). There are some optimization tools currently in development to support operational and strategic planning as well as infrastructure build-outs (e.g., NETL 2022). However, many oil producers use qualitative strategies to assess ESE tradeoffs (often referred to in a slightly different manner in the oil and gas industry as environmental, social, and governance (ESG)) since there is no comprehensive tool for **quantitatively** assessing the full ESE costs and benefits of supplementing limited freshwater resources in many oil and gas regions with alternative produced water treatment, management, and reuse strategies (Danforth et al. 2019). In fact, the Environmental Protection Agency (EPA) through their Water Reuse Action Planning efforts have identified produced water reuse for fit-for-purpose uses outside the oil and gas sector as a potentially important source of new water but which requires improved tools for socio-economic, environmental, ecological risk and toxicology cost benefit analyses (USEPA 2020).

1.2. Goal

The goal of this work is to *develop an integrated model for assessing the economic, societal, and environmental tradeoffs associated with alternative produced water management and fit-for-purpose treatment and reuse strategies related to oil and gas development and production*. The tool is intended to be easy to use, quantitative tool that can be tailored to the unique characteristics of an oil/gas project and locale. Considerations will include both source water selection as well as produced water treatment, application, and disposition. The model user interface will be designed to support diverse stakeholders, including producers, technology developers, economic development agencies, and regulatory agencies to help inform the development of sound science-based decisions on the reuse of treated produced water for maximum societal and economic benefits while protecting public, environmental, and ecological health and safety.

1.3. Project Overview

A proof-of-concept, easy to use analysis tool, the Produced Water-Economic, Socio, Environmental Simulation model (PW-ESESim) was developed. The tool was designed to facilitate head-to-head comparison of alternative produced water source, treatment, and reuse water management strategies. A graphical user interface (GUI) guides the user through the selection and design of alternative produced water treatment and reuse strategies and the associated health and safety risk and economic benefits. At the highest conceptual level, alternative water strategies include the selection of a source water (locally or regionally available produced water), treatment strategy (pre-treatment, physical, chemical, biological, desalination, and post-treatment processes) and product water purpose (e.g., irrigation, industrial processing, environmental). PW-ESESim assists the user in identifying the resulting impacts on key ESE as well as public/ecological health and safety metrics; specific examples include, cost of treatment, improvements in freshwater availability, human and ecologic health impacts and growth in local jobs and the economy. Through the simulation of different produced water treatment and management strategies, tradeoffs are identified and used to inform fit-for-purpose produced water treatment and reuse management decisions. While the tool was initially developed using oil and gas produced water treatment and reuse management details from Southeastern New Mexico (Permian Basin) as a case study, the PW-ESESim model serves as a proof-of-concept platform and serves to inform future extensions to other oil and gas regions of the U.S.

1.4. Potential Impact

This project resulted in the development of a first-of-its-kind, proof-of-concept tool for quantitatively assessing the economic, social, and environmental tradeoffs associated with alternative treated produced water management strategies. PW-ESESim is also designed to be broadly accessible and of immediate value for a range of uses:

- Oil and Gas Industry - provides a quantitative triple-bottom-line assessment for treated produced water project design and evaluation.
- EPA supported efforts of the National Water Reuse Action Plan - provides a much needed analysis tool for treated produced water reuse nationally. Additionally, this tool could be expanded to reuse assessments for other non-traditional energy-water source waters such as for thermoelectric power plant cooling and blowdown water treatment and reuse.
- Water and Economic Developers - assisting developers of industrial, municipal, mining, and agricultural projects in evaluating treated produced water as a potential source water for enhanced economic development locally, as well as guiding selection of competing treatment and concentrate disposal options.
- Regulators - provides a means for initial assessment of proposed oil and gas produced water treatment and reuse policies and projects.
- Land Managers - supports necessary water-related assessments prior to extending or issuing new oil and gas leases.
- Public and environmental groups - provides a quantitative tool for communicating complex environmental and ecological risk and toxicology-based decisions on the treatment and reuse of produced to the public.

2. MODEL ARCHITECTURE

Selection of an appropriate architecture for this modeling exercise was based on two criteria. First, a model was needed that provided an "integrated" view of the problem — one that couples the complex physics of oil and gas produced water treatment, management, and reuse with its diverse impacts on the regional economy, society, and the environment. Second, a model was needed that can be taken directly to a wide range of stakeholders to support specific decisions, enhance risk communication and provide an educational tool. For these reasons we adopted an approach based on the principles of System Dynamics (SD) (Forrester 1990; Sterman 2020).

According to this architecture, PW-ESESim is organized according to a series of interacting modular systems focused on engineered, economic, societal, environmental, and health and safety systems (Figure 1). In turn, each system is composed of a series of interacting subsystems. These systems and subsystems are each quantified by traditional dynamical models of key physical/social processes.

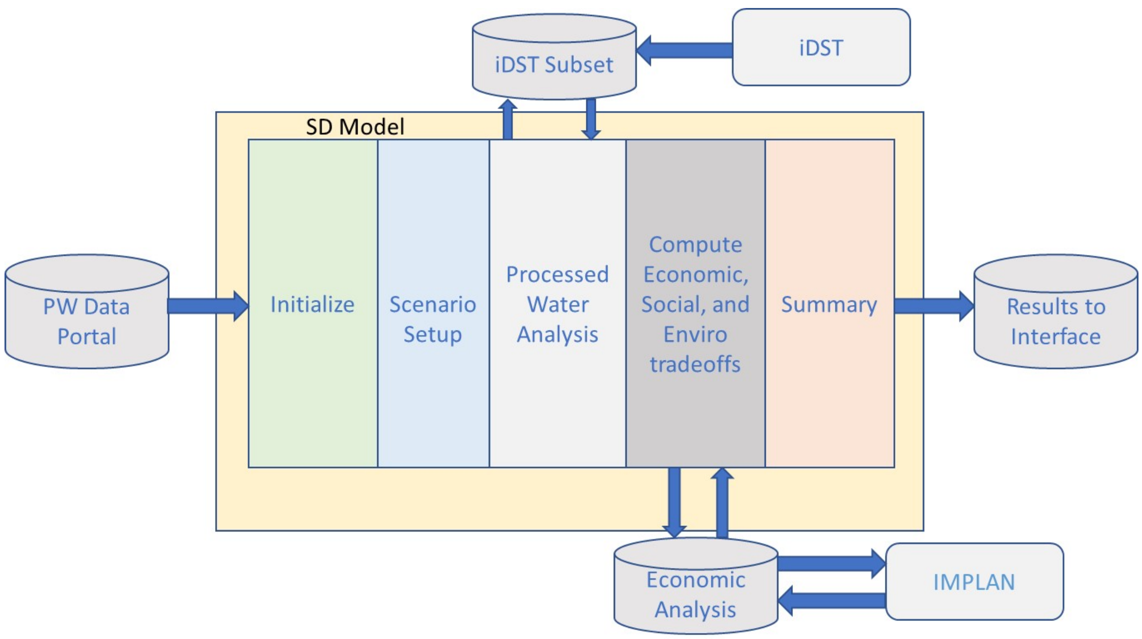

Figure 1. Schematic of PW-ESESim model layout. iDST = integrated Decision Support Tool.

Modeled processes capture critical feedbacks that selected produced water treatment and management strategies have on ESE systems. There are many feedbacks as multiple source waters are considered (various treated produced waters, recycled wastewater) as well as multiple options for treated produced water disposition; specifically, deep well injection, on onsite uses for hydraulic fracturing and drilling, as well as other fit-for-purpose beneficial uses (agricultural irrigation, in-stream flow augmentation, and other user defined options). Ultimately, the value of this approach is that each of system/subsystems are modeled endogenously, that is fully interacting with one another.

In this application, the SD-based PW-ESESim model operates in a geospatial context resolved at the quarter-township scale (~9 mi^2). Analysis focuses on a particular locale to evaluate tradeoffs that can be aggregated to regional scale. The case study used for the modeling domain encompasses Lea and Eddy Counties in Southeastern New Mexico (Figure 2), an area of prolific oil and gas production. The simulation proceeds in monthly timesteps up to a multi-decadal time horizon. This spatiotemporal approach provides critical insight into how the integrated systems co-evolve and identifies critical time dependencies across interacting systems.

PW-ESESim can be used to perform tradeoff analysis by adjusting key exogenous factors (e.g., oil production rates, produced water disposal costs). This analysis is accomplished through an easy-to-use graphical user interface that includes slider bars and radio buttons that allow the analyst to try alternative source and produced water treatment and reuse and management strategies. Through this same interface, results are rendered to a variety of tables, graphs, and maps for evaluation. Execution of the simulation is very efficient (few tens of seconds to a few minutes), allowing for rapid scenario testing at one's desk or in a stakeholder workshop setting.

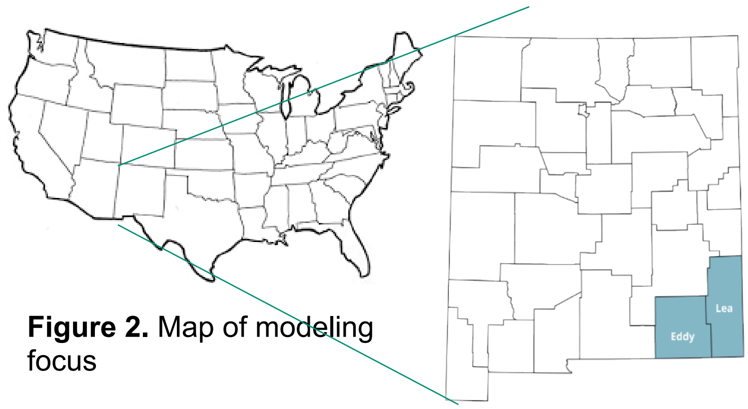

Figure 2. Map of modeling focus

A key feature of the model building process was extensive interaction with a range of stakeholders; particularly, industry, regulators, water developers among others. This team of stakeholders was engaged to aid in conceptual model development, identification of critical data sets, defining model specifications and, in final vetting of the model's performance. Stakeholder engagement was accomplished by way of virtual workshops plus other ad hoc meetings and communications as required. A series of project-end workshops allowed stakeholders to test specific real-world problems and give feedback on the efficacy of the model. The New Mexico Produced Water Research Consortium (NMPWRC) served as the convener, providing direct access to an extensive stakeholder team including Groundwater Protection Council (GWPC); NMTech and their Petroleum Recovery Research Center; various state agencies (NM Department of Agriculture, NM State Engineer, NM Department of Health, NM Environment Department, NM Oil Conservation Division (NMOCD) of EMNRD); as well as local and regional economic development groups. In addition, NMPWRC provided access to over 100 member groups including producers, midstream companies, academics, consultants, vendors, and state and federal agencies across Oklahoma, Texas, and Wyoming.

The following section contains detailed description of the system submodels.

3. OIL AND GAS MODEL

This submodel addresses the engineered system associated with oil and gas development. This system is limited to those elements that influence the production and disposition of produced water, namely:

- Oil and gas/produced water production
- Source water for oil and gas development
- Produced water treatment
- Wastewater disposal, and
- Transport of produced water

Each of these elements are discussed in greater detail in the following subsections.

3.1. Oil and Gas/Produced Water Production

There is no clear reason to model actual gas/oil production. Rather, the economic output of the oil/gas industry (see Economic submodel) was used as a proxy for these values. Current economic production numbers by county are available while future economic production is scaled to changes in source water demands for oil & gas development (see below). Also computed are the overall costs related to produced water management. Additionally, the economic production values are adjusted based on the change in costs for produced water management (see Economic submodel for more details).

More precision is required for produced water production. Two data sets were merged to create a detailed accounting of produced water production. First, produced water historically disposed in salt water disposal wells was taken from the New Mexico Produced Water WaterSTAR Data Portal[1] developed by the Groundwater Protection Council. This data set included historical volumes of produced water and water quality data limited to total dissolved solids (TDS) and some of the major ions. The data were organized by township parcels. For each township monthly production rates were averaged from 2015-2020. Second, the New Mexico Recycling Facilities Database, collected by NMOCD, provided data to help locate and determine the quantity of produced water that is treated and recycled in oil and gas production[2]. NMOCD recognizes that this database is incomplete, which agreed with comparisons that we drew between this dataset and statewide projections of produced water reuse (NMOCD's Water Use Summary Report; see below for more details) that disagreed by an order of magnitude. As such, estimates of reused produced water for oil and gas development was approached in a different way (see Section 3.2). Total produced water volumes were then estimated by adding the salt water disposal volumes with the produced water reuse values.

Given the limited availability of produced water quality data and the screening-level purpose of the model, water treatment decisions were based on TDS data, which is available at the township level. Data were available only through 2015 so aggregated values were constructed over available monthly data from 2011-2015. Other constituent levels are based on basin-wide estimates, which scale with the TDS level.

Future production rates and chemistry are not expected to vary significantly from month to month as produced water is mixed from numerous wells. However, production rates are expected to grow in the future as new wells are drilled. It is assumed that production will scale directly with the increase in oil & gas development. If new development stalls due to a market downturn, produced water

[1] https://waterstar-nm.cstestsite.com

[2] https://www.emnrd.nm.gov/ocd/ocd-data/statistics/

production rates will be kept constant over this period to reflect continued production from existing wells.

3.2. Source water for oil and gas development

In this submodule, the location, volume, and source of water used in oil & gas development (drilling and stimulation) is simulated. This includes current water use as well as projections for future use.

Two sources of data were compiled to estimate current use characteristics. State-level data on a monthly basis was collected from NMOCD's Water Use Summary Report[3]. Included are volumes of water used and type of source water (fresh, brackish, produced, saline). An important limitation is that collection of this data only started in October 2020. This dataset will be extended by using the Frac Focus chemical disclosure registry[4]. This dataset substantially increases the time period of data and includes water use volumes and well locations—however, it doesn't include a source water descriptor.

Characterization of current water use requires estimation of the volume, source, and location of the demand. To do this we began by comparing the state-level projections from OCD with oil & gas water use values from Frac Focus combined over Lea and Eddy Counties (where the majority of water is used for oil and gas development in the state). The Frac Focus totals tended to be a little higher (14%) than the state-wide number from the OCD. Given the comparability of the two datasets and the lack of a better alternative, we adopted the Frac Focus data to map out oil & gas water demand by township. Current water demand, data collected between 2018 and 2020 were averaged (note that there was a steep growth in demand prior to 2018). An average was taken over this period to address annual variations in activity.

From the Frac Focus data, total water demands by location (township/range) were estimated. The next step was to identify the source water. The only information available is the state-level data from the OCD and limited specific data for Lea and Eddy counties. Using the state and limited county level data, the mix of source waters was determined (see Table 1). The mix ratios were applied uniformly by county—with one exception. Township elements that overly the Capitan Underground Water Basin were not assigned any fresh groundwater use as very limited freshwater is available in this region.

Table 1. Source Water Mix Ratios

Source Water	Eddy	Lea
Produced Water	0.42	0.40
Brackish Water	0.50	0.45
Fresh Water	0.08	0.15

Again, future production rates are dictated by user input. While the model user can adjust growth rates as desired a single hard-wired option is offered. This growth rate is based on growth in water use for oil & gas development as taken from the Frac Focus data set (see above). Over the last four years (2018- mid 2021) a steady growth of 450 af/yr of water demand across each county has been realized. This equates to a growth rate of 3%. A couple of other points of reference were in the regional water plans, which project growth in water demand for oil & gas. However, their projections from 2010-2020 significantly underpredicted reality. A report by Scanlon et al. (2020) suggest the Delaware Basin could have an additional 80 years of life and water demands could double.

[3] https://wwwapps.emnrd.state.nm.us/ocd/ocdpermitting/Reporting/Wells/WaterUseSummaryReport.aspx

[4] https://fracfocus.org/data-download

Along with the quantity of water used in the oil & gas sector is the cost associated with the water accessing the water for drilling and stimulation. Here a simple price per barrel of water is used which varies by source. Based on feedback from our local stakeholders, freshwater is assumed to be leased at $1/barrel while brackish groundwater costs about $0.6/barrel. The default cost to treat and recycle produced water is set at $0.50/barrel within the model. However, all costs can be adjusted by the model user.

3.3. Produced Water Treatment

Necessary levels of produced water treatment are modeled using the integrated Decision Support Tool (iDST) (Geza et al. 2018; Ma et al. 2018). iDST is designed to select produced water treatment processes using a constrained multi-objective optimization (MOO) approach. Selection follows user defined objective functions and constraints based on water quality, costs, energy, and other technical criteria. The iDST includes 62 standalone and hybrid configurations of treatment technologies and their removal capacities for each water quality constituent for the selection of pre-treatment, physical, chemical, biological, desalination, and post-treatment processes. Beyond proposing a specific treatment train, the iDST calculates system costs based on the selected treatment technologies, desired product water flow rate, and economic inputs assigned by the user, and outputs unit cost, and annual capital cost, operation and maintenance (O&M) costs, and energy consumption.

To estimate levels of produced water treatment, three key data inputs are required: produced water quality, total system through put, and product water quality. It was realized that the viable produced water reuse options for southeastern New Mexico resulted in the need to simulate a relatively small number of water treatment scenarios. Specifically, twenty-seven scenarios were found to adequately span the range of treatment options. These were selected to both span the range of reuse options as well as the non-linear scaling of technology costs across capacity and treatment levels. Treatment scenarios were organized according to the following 3x3x3 matrix:

1. Produced water quality
    a. Low: <40,000 mg/L (25,000 mg/L)
    b. Medium: 40,000 – 100,000 mg/L (100,000 mg/L)
    c. High: >100,000 mg/L (150,000 mg/L)
2. Treatment capacity
    a. 5000 billion barrels of petroleum liquids per day (bbl/d)
    b. 20,000 bbl/d
    c. 50,000 bbl/d
3. Beneficial use scenarios
    a. Applications that require drinking water quality (i.e., potable water), such as groundwater recharge (TDS 500 mg/L)
    b. Ag irrigation / stream augmentation, range lands (2000 mg/L)
    c. Clean brine for hydraulic fracturing (oil and gas), industry (e.g., potash mining)

As we were able to distill the viable treatment options into a manageable number of scenarios, it was not necessary to couple iDST directly with PW-ESESim. Rather, the 27 simulations were performed offline with iDST and results were organized into an Excel worksheet that was linked to PW-ESESim. iDST results that captured in the database and subsequently used by PW-ESESim include:

- Proposed treatment train,
- Capital cost,
- Annualized capital cost,

- Total annual O&M costs,
- Total energy demand,
- Water recovery, and
- Normalized cost per barrel of treated water

As noted above, produced water quality data beyond TDS is very limited. To fill in this gap, we collected produced water samples from salt water disposal wells in the Permian Basin, and used the average concentrations of different constituents to develop produced water quality profiles that varied according the TDS level. These profiles are provided in Table 2.

Assumed product water quality standards are based on the National Primary and Secondary Drinking Water Regulations set by the USEPA Safe Drinking Water Act (SDWA), Irrigation Guide by US Department of Agriculture (USDA, 2011 and 1993), New Mexico state regulations (NMAC, 2020), and emerging industry standards for clean brine (Horn, 2019). The standards for the three product water quality scenarios are included in Table 2.

3.4. Wastewater Disposal

Wastewater disposal applies to both any unused produced water as well as any concentrates produced by way of produced water treatment. As noted above, we have good data on the location of salt water disposal wells and the amount of produced water currently being injected (New Mexico Produced Water WaterSTAR Data Poral). This disposal volume will change over time based on the amount of produced water treated; that is, disposal volume is reduced by the treated volume recovered. Disposal will also change based on growth in oil & gas production.

Beyond the modeling of changes in disposal volumes, efforts are made to estimate the cost of disposal. Through our stakeholder engagement process, we received a range of estimates on disposal costs for SE New Mexico ($0.5 - $1.5/barrel). This range reflect the variety of factors influencing costs, including contracting between producer and the disposal company. Long term contracts generally result in lower costs. In SE New Mexico, cost appear between. We adopt a value of $0.75/barrel but allow the user to adjust this value. Also, the costs are expected to rise over time as has been the trend over the last 20-years. Following this historical trend, a growth factor in cost of $0.063/barrel year is adopted here.

3.5. Wastewater Disposal

Based on feedback from stakeholder engagement efforts, it is apparent that the majority of produced water transport occurs via permanent underground pipelines. Approximately 25% is transported by truck, primarily from regions with sparse oil & gas activity but trucking is also used to handle large initial flowback volumes following "on-lining" of a new well. Of primary interest to our modeling are the costs associated with produced water transport, which include the construction of pipelines and operational expenses of trucking.

Table 2. General Water Quality of Different Produced Waters Expected to Be Treated (based on general New Mexico produced water quality data) and General Product Water Quality in Different Beneficial Scenarios. All values are in mg/L except for Temperature (oC) and Turbidity (NTU)

	Low TDS PW	Medium TDS PW	High TDS PW	Potable use, aquifer recharge	Crop irrigation	Clean brine
Alkalinity (as CaCO3)	180	900	1300	-	-	-
Aluminum	1	3	4	0.200	5	-
Ammonia	300	600	99	2	-	-
Barium	1	3	4	2	-	-
Benzene	170	170	170	0.005	-	-
Boron	5	20	30	-	0.750	-
Bromide	120	650	950	-	-	-
Calcium	500	2500	3800	-	-	-
Chloride	12,000	60,000	90,000	250	110.0	-
Ethylbenzene	100	100	100	0.700	-	-
Iron (III)	10	40	60	0.300	5	20.0
Lithium	1	6	10	-	15	-
Magnesium	100	400	600	-	-	-
Manganese	0.10	1	1	0.050	0.200	-
Oil and Grease	80	80	80	-	-	30.0
pH	6.80	6.80	6.80	-	6-8	6-8
Silica (SiO2)	2	10	15	-	-	-
Sodium	7,000	35,000	50,000	-	-	-
Strontium	50	300	400	-	-	-
Sulfate	150	800	1200	250	-	1000.0
TDS	25,000	100,000	150,000	500	1500	-
Temperature	38	38	38	-	-	-
Toluene	2	2	2	1	-	-
Total Organic Carbon (TOC)	150	150	150	-	-	-
Turbidity	50	50	55	0.300	-	25.0
Uranium	0.20	0.50	0.50	0.030	-	-
Zinc	0.60	1	1	5	-	-

Pipeline Transport: Current cost for produced water transport via pipelines is $0.25/barrel (feedback from local stakeholders). This cost is assumed for all produced water except that which is trucked (e.g., ~25%), this includes any growth in production due to addition of new oil & gas wells. New pipeline costs are assessed only to deliver the treated water. We assume treatment will occur at the disposal site to take advantage of the existing network. Costs then are incurred to build a pipeline between the treatment facility and the final point of use. For beneficial reuse projects pipeline costs, C_{pl}, are the product of the pipe diameter, *dia*, pipe length, *l*, and cost factor, *CF*:

$$C_{pl} = CF * dia * l \quad (1)$$

The cost factor is set at $10, while the diameter depends linearly on the flow rate (6 inch for 0.15 MGD to 12 inch for 1.5 MGD; not to exceed 36 inch). The length varies by township and is assumed to be the average distance between salt water disposal wells and the township centroid. If the project requires transport beyond the township, the distance between township centroids is added.

Trucking Transport: Cost for truck transport depends on how much water is moved. There are no data characterizing the volumes of water trucked in each township. As such, we assume townships with really low produced water production are not piped. A cutoff of 5 million gallons/month appeared to capture the majority of townships with sparse oil & gas wells. However, the total volume of produced water production in these sparse townships was less than 1% of the total production. As such, from the remaining townships, 24% (or 1% less than that specified by the model user) of the total produced water production is assumed to be trucked (assumed associated with transport of high capacity flows following initial production of a new well).

Trucking cost also depends on the distance it is moved, TD_i. Again, the average length between the oil & gas wells and the salt water disposal well is used (l_i, where i is the township). This distance is increased by a factor of 1.5 to account for the difference between straight line and road distance. This distance is then doubled to account for coming and going between well and disposal. The distance also depends on the number of trips, which accounts for fact that New Mexico limits transport volumes to 120 barrels. Together the distance calculation takes the form:

$$TD_i = l_i * 1.5 * 2 * \left(\frac{PW_i}{120}\right) \quad (1)$$

To get the transport cost, TC_i, we convert the distance to time assuming a maximum speed to 40mph and a cost of $90/hr:

$$TC_i = \left(\frac{TD_i}{40mph}\right) * \$90/hr \quad (2)$$

Note that the parameters supplied above were acquired from conversations with local stakeholders; however, these values can be adjusted by the model operator. Where piping replaces trucking we will assume transport costs equal $0.4/barrel to capture the added expense of managing these more difficult waters. We also assume that trucking will always be necessary for at least 10% of all produced water generated.

Truck traffic is also of concern for evaluating impacts to environmental justice. Here we track changes in the total miles of trucked produced water (TD_i) as an input to justice calculations (see Section 7).

4. HYDROLOGY MODEL

This submodel addresses all potential source waters in Lea and Eddy counties, including:

- Fresh groundwater,
- Fresh surface water (Pecos River),
- Brackish groundwater,
- Reclaimed wastewater, and
- Produced water.

The overarching purpose of the model is to track how water use choices impact the supplies of alternative sources of water (e.g., how new demands are sourced). Key demand sectors include:

- Oil & Gas,
- Agriculture,
- Municipal,
- Industrial/Commercial/Mining/Power (ICMP), and
- Domestic/Livestock.

The model user has the option to control how water demands change over time and how those new demands are allocated. These choices will be input to other portions of the model, particularly the economic submodel in terms of water costs and tradeoffs in the economy (e.g., new industrial growth, added crop land). Below we break down the modeling for each water source, but first we address modeling of water demand.

4.1. Water Demand

Current water use conditions in the basin form the baseline for the analysis. Water use as reported in the most recent Regional Water Plans (2010) (https://www.ose.state.nm.us/Planning/rwp.php) were compared to the 2015 USGS Water Census (Dieter et al. 2018). Estimates were relatively similar so the USGS data were adopted (Table 3). Demands are characterized on the basis of water withdrawals, across the five demand sectors noted above.

In each sector, the demand is further distinguished on the basis of source water and point of diversion. For example, water used in the oil and gas industry is predominately from brackish and recycled produced water with minor use of fresh water; use data is captured by NMOCD (described in Section 5). Agricultural water use statistics are available at the county level from the Regional Water Plans and USGS Water Census. Water use is then spatially distributed according to land use classifications by township (land use/land cover data described in Ma (2020). Municipal water use data by community is given in the Regional Water Plans. Self-supplied ICMP data as well as domestic/livestock are available at the county level from the Regional Water Plans and USGS Water Census. ICMP demands are spatially distributed according to the NM Water Rights Reporting System (https://www.ose.state.nm.us/WRAB/), while domestic water use is distributed by relative acreage in ranching and farming.

Table 3. Water withdrawals by county (Dieter et al. 2018). Values in AF/yr

Use Category	Lea	Eddy
Public Supply	11,409	15,059
Domestic/Livestock	4377	1545

Irrigation	165,895	89,884 plus 65,975 from Pecos
ICMP	5094	3303

From the 2015 baseline, there is interest in projecting changes in demands and or the sourcing of new and/or existing demands. A growth scenario is offered that is patterned after projections in the Regional Water Plans (Table 4). The user also has the option to project their own new growth rates. Beyond the growth rate, the user could select the mix of water sources that are tapped. Specific details/constraints for each sector are as follows:

- Oil & Gas: the base growth scenario will be patterned after historical trends in water use. The user can increase or decrease the trend as well as adjust the mix of fresh/brackish/produced water used for new fracking jobs (at the county level).
- Agriculture: Agriculture in the region is not projected to increase without a new water source. Here the user will have the option to click on a location to add new irrigated acreage watered with treated produced water or change current sources from freshwater to treated produced water.
- Municipal: User can adopt the growth projection or choose their own; they can also choose whether the new water supply is sourced from fresh or brackish water (or both).
- ICMP: User can adopt the growth projection or choose their own by county. Will also have the option to choose whether the new water supply is sourced from fresh, brackish, reclaimed wastewater, or treated produced water (or a mixture of the four).
- Domestic/Livestock: User can adopt the high or low growth projections or choose their own for each county. Will assume growth will be served from fresh groundwater.

As an example, a user could decide, for a given region i, that the generation of produced water will grow at a particular rate ($\Delta PW_{prod,i}^{t}$) and chooses to reduce the amount of brackish water used in oil and gas development ($\Delta Brack_{O\&G,i}^{t}$), while increasing the use of produced water for oil & gas ($\Delta PW_{O\&G,i}^{t}$) and agriculture ($\Delta PW_{ag,i}^{t}$).

Table 4. Projected growth rates by county and sector captured as defaults within the model. Growth rates in AF/yr. Data taken from the Regional Water Plans.

	Lea		Eddy	
	High	Low	High	Low
Municipal	178.94	83.82	118.18	71.5
Domestic/Livestock	26.7	5.82	No growth	No growth
Irrigation	No growth	No growth	No growth	No growth
ICMP	8.46	No estimate	No growth	No growth

4.2. Fresh Groundwater

There will be no attempt to develop a groundwater model for the region as this is beyond the scope and need of this screening tool. Rather, a water use budget approach will be taken where the focus will be on projecting changes in water use with time. It is important to note that all declared underground water basins in Lea and Eddy Counties are closed to new appropriations except for domestic and livestock permits. However, the purpose and point of use of existing water rights can be changed. As such, the pumping rates are fixed except for small projected growth in domestic and livestock uses.

Water use budgets were developed for each declared Underground Water Basin in Lea and Eddy Counties—Lea County (Ogallala), Jal, Carlsbad, Capitan, and Roswell. The water use budget will take the following form where we assume that any projected growth in fresh groundwater use will be met by an equal decline in agricultural water use:

$$Fresh_{ag,i}^{t} = Fresh_{ag,i}^{t=0} - \left(\Delta Fresh_{muni,i}^{t} + \Delta Fresh_{ICMP,i}^{t} + \Delta Fresh_{O\&G,i}^{t}\right), \quad (3)$$

where:

$Fresh_{ag,i}^{t}$ = Fresh groundwater use in agriculture in region *i*, at time *t*

$Fresh_{ag,i}^{t=0}$ = Fresh groundwater use in agriculture in region *i* at the initial time step

$\Delta Fresh_{muni,i}^{t}$ = Change in fresh groundwater use in the municipal sector in region *i*, at time *t*

$\Delta Fresh_{ICMP,i}^{t}$ = Change in fresh groundwater use in the ICMP sector in region *i*, at time *t*

$\Delta Fresh_{O\&G,i}^{t}$ = Change in fresh groundwater use in the oil and gas sector in region *i*, at time *t*.

All terms are in units of volume/time. Note that all the delta terms are user specified and incrementally grow over time according to the use scenario (high/low/other). However, the change in freshwater use in the oil & gas sector is implemented over a defined time horizon consistent with the time to construct the necessary infrastructure (assumed 5 years). Here we are also assuming that freshwater use by oil & gas is exchanged directly with agricultural use; that is, if oil & gas reduces freshwater use then that water will be used in ag and vice-versa (assuming oil & gas leases their water from agriculture). The overarching water use budget then takes the form:

$$Fresh_{tot,i}^{t} = Fresh_{tot,i}^{t-1} + \Delta Fresh_{DL,i}^{t} - \Delta Fresh_{ag,i}^{t} \quad , \quad (4)$$

where:

$Fresh_{tot,i}^{t}$ = Total fresh groundwater use in region *i*, at time *t*

$Fresh_{tot,i}^{t-1}$ = Total fresh groundwater use in region *i*, at time *t-1* or prior time step

$\Delta Fresh_{DL,i}^{t}$ = Change in fresh groundwater use in the domestic and livestock sector in region *i*, at time *t*

$\Delta Fresh_{ag,i}^{t}$ = Change in fresh groundwater use in the agriculture sector in region *i*, at time *t*. Note that this only applies to user specified decreases in agriculture, generally due to offsetting use of treated produced water

Again, all in units of volume/time. Note that $Fresh_{tot,i}^{t}$ accumulates over time (i.e., create a stock and accumulate the total water surplus or deficit). None of the other water use budgets accumulate over time.

4.3. Brackish Groundwater

Unlike fresh groundwater, there are no administrative controls on brackish water use (nor do we expect any physical controls will limit use). Again, a water use budget approach is used which takes the form:

$$Brack_{tot,i}^{t} = Brack_{tot,i}^{t-1} + \Delta Brack_{muni,i}^{t} + \Delta Brack_{ICMP,i}^{t} + \Delta Brack_{O\&G,i}^{t} \quad (5)$$

Terms follow similar naming convention as above (all in units of volume/time). Again, all delta terms are defined by the user and incrementally grow over time according to the use scenario (high/low/other). However, the change in brackish water use in the oil & gas sector is implemented over a defined time horizon consistent with the time to construct the necessary infrastructure (assumed 5 years). Note that brackish water use in the oil & gas sector could go up or down.
Currently there is little brackish water use outside of oil and gas, within Lea and Eddy counties. The one exception is potash mining which we have no way of estimating.

4.4. Reclaimed Wastewater

Reclaimed wastewater supply is limited by the amount of wastewater that is produced and captured by a treatment facility. The water use budget takes the form:

$$WW_{avail,i}^{t} = (WW_{avail,i}^{t-1} + \left(\Delta Fresh_{muni,i}^{t} + \Delta Brack_{muni,i}^{t}\right) * WWF\big) - \Delta WW_{ICMP,i}^{t} \quad (6)$$

Where:

$WW_{avail,i}^{t}$ = The wastewater available for use in region *i*, at time *t*

$WW_{avail,i}^{t-1}$ = The wastewater available for use in region *i*, at the previous time step *t-1*

WWF = The portion of the municipal water withdrawal that is returned to the wastewater plant (65% is adapted based on long term averages from USGS).

$\Delta WW_{ICMP,i}^{t}$ = Change in reclaimed wasted water use in the ICMP sector in region *i*, at time *t*.

All in units of volume/time except WWF which is dimensionless. Again, all delta terms are defined by the user and incrementally grow over time according to the use scenario (high/low/other). Also calculated is the reclaimed wastewater that is being used which is determined by simply summing $\Delta WW_{ICMP,i}^{t}$.

Wastewater production data was taken from the regional water plans. Data was distributed by township and range. There is no current indication of any recycling of local wastewater.

4.5. Produced Water

The water use budget (estimated by county) for produced water is calculated as:

$$PW_{tot,i}^{t} = MIN\left[(PW_{prod,i}^{t-1} + \Delta PW_{prod,i}^{t}), \left(\Delta PW_{ag,i}^{t} + \Delta PW_{ICMP,i}^{t} + \Delta PW_{O\&G,i}^{t}\right)\right] \quad (7)$$

Where: all in units of volume/time

$PW_{tot,i}^{t}$ = The total produced water put to beneficial use in region *i*, at time *t*

$PW_{prod,i}^{t-1}$ = The total produced water generated in region *i*, at time *t-1* or the previous time step

$\Delta PW_{prod,i}^{t}$ = The change in produced water generated in region *i*, at time *t*

$\Delta PW_{X,i}^{t}$ = The change in produced water use by sector in region *i*, at time *t*

The MIN function is simply used to prevent the new demands for produced water from exceeding the produced amount. All delta terms are defined by the user. The production term grows incrementally over time, while the use terms are implemented over a defined time horizon consistent with the time to construct the necessary infrastructure (assumed 5 years). More details about produced water generation is captured in Section 3.

4.6. Fresh Surface Water (Pecos River)

Operations of the Pecos River are very complex and hence beyond the ability to model at a scoping level. Nevertheless, the value of adding treated produced water to the Pecos is assessed. In discussions with Pecos River water managers, we were informed that there is little need for the water to meet downstream compact requirements with the State of Texas. As such, water added to the river would fulfill one of two purposes. First, the treated produced water would help augment flows for environmental services. However, the amount of water is small relative to the natural flow of the river. A single project (50,000 bbls/d) would add ~1.62 cfs to the river, which has an annual average stream flow of 165cfs (this water could be managed in Brantley Reservoir to meet environmental flow targets during unseasonable low flows alternatively). The second, more likely purpose for the water would be use by the Carlsbad Irrigation District. This would represent about 1200 AF of water to a district that uses 66,000 AF of water per year from the Pecos.

4.7. Total Change in Beneficial Water Use

The total water put to beneficial use in the model is calculated as:

$$Q^t_{tot,i} = Fresh^t_{tot,i} + Brack^t_{tot,i} + PW^t_{tot,i} + \sum_{t=0}^{t} \Delta WW^t_{ICMP,i} \qquad (8)$$

5. ECONOMICS

The economics framework is built upon a macro-economic model using the commercial software IMPLAN (2021). The IMPLAN model is an input-output model that looks at the interdependencies between economic sectors. Within the study area (Lea and Eddy county), for instance, an increase in oil and gas mining could result in an economic gain to other industries that depend upon oil and gas or support oil and gas such as trucking and transport, road maintenance and residential growth. The outputs from this model demonstrate the dependency between sectors of an economy.

A strength and weakness of an input-output model is that it is linear in nature, this allows for rapid computation and flexibility in computations. However, if the interdependencies between sectors are not linear in nature, an input-output model cannot account for this structure. Figure 3 demonstrates the theoretical flow of the economic model. The IMPLAN model is able to calculate economic benefits to sectors of the economy at the macro level.

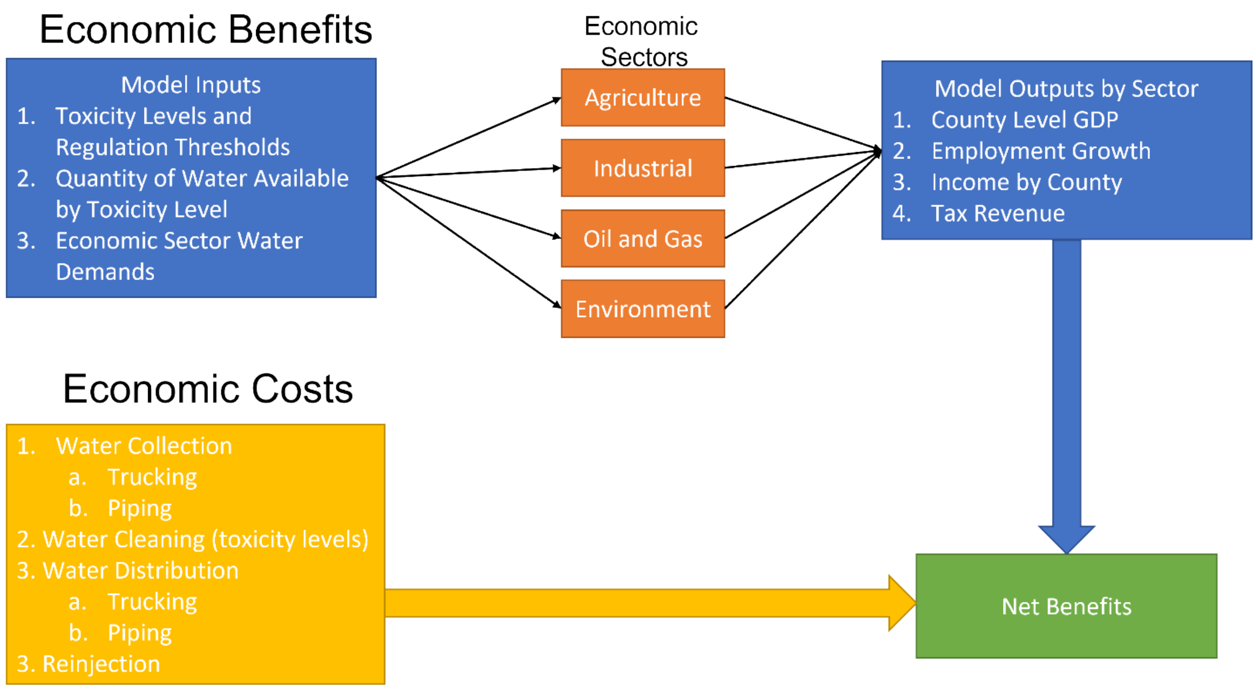

Figure 3. Schematic of economic systems model as implemented within PW-ESESim.

Table 5 displays the current economic conditions (i.e., baseline) in Lea and Eddy counties. The IMPLAN model has over 500 economic sectors that can be tracked at the county level. Twenty-six sectors are shown in Table 5 as a point of reference. As a sector's production level is increased (due to more water being available as an input to the sector), the IMPLAN model will report the changes to other sectors as resulting from these changes. This creates the economic benefits from Figure 3.

Ten sectors are targeted as industries with the potential to grow due to access to treated produced water. These include grain farming; all other crop farming (direct use of treated produced water or through discharge and later capture from the Pecos River); tree nut farming; beef production; petroleum refineries; potash, Soda and Borate mining; and data centers; manufacturing; and crop grown for carbon sequestration. Using data from the baseline model (Table 5) the current economic value of each of these sectors is known. Water use data from the USGS Water Census and NM

Table 5. Economic Baseline (2019) Values for the Two Counties Used in the Case Study

	Lea	**Eddy**
Year	2019	2019
Population	71,070	58460
Employment	42,931	42,370
Households	24,870	22,274
Number of Industries	219	224
Output	**$11,371,733,109.45**	**$13,255,494,023.61**
Petroleum refineries (154)	$1,701,018,709.52	$2,031,646,600.35
Oil and gas extraction (20)	$1,485,051,628.79	$2,843,265,088.37
Support oil and gas (36)	$1,472,959,279.30	$1,553,607,229.90
Drilling oil and gas (35)	$808,963,799.61	$199,653,274.53
Truck Transportation (417)	$378,795,634.15	$249,368,960.42
Potash soda and borate (31)	$42,604,703.40	$186,723,308.31
Metal Mining (37)	$150,465,910.44	$316,096,586.44
Plastics pipe and pipe fitting manufacturing (188)	-	$85,169,695.44
Ready-mix concrete (204)	$5,163,189.96	$46,749,168.65
Grain Farming (2)	$1,636,121.49	$1,739,330.43
Tree nut farming (5)	$4,483,700.68	$20,131,466.78
All other crop (10)	$17,109,017.29	$19,538,386.93
Dairy Cattle and milk (12)	$135,590,690.21	$36,494,504.57
Beef Cattle ranching (11)	$64,361,679.78	$26,361,063.63
Construction of highways and streets (54)	$52,382,836.20	$53,024,065.51
Construction of new manufacturing (51)	$27,956,647.13	$27,414,251.43
Power and transmission (47)	$156,428,560.27	$219,700,566.88
Wholesale Machinery Equipment and supplies (395)	$118,791,342.50	$105,174,049.00
Retail Gasoline stores (408)	$20,631,079.17	$58,535,613.15
Retail General Merchandise (411)	$54,161,191.22	$56,647,954.53
Hospitals (490)	$127,892,636.10	$171,821,432.72
Full service restaurants (509)	$57,648,686.20	$65,118,204.37
Local government education (542)	$158,974,595.15	$110,039,521.09
Water sewer and other systems (49)	$2,668,271.85	$22,822,107.32
Construction of new power and communication (52)	$121,755,934.41	$125,540,865.63
Construction of single family residence (57)	$118,914,310.99	$117,942,946.44
Value Added (GDP)	**$5,988,885,717.74**	**$7,593,747,168.19**
Employee Compensation	$2,522,451,767.30	$2,825,860,351.46
Proprietor Income	$363,961,674.85	$184,401,716.23
Other Property Income	$2,447,875,785.99	$3,852,781,464.56
Taxes on Production and Imports	$654,596,489.61	$730,703,635.93

Water Rights Reporting System the associated water use with each sector is also determined. We assume that this ratio between water use and economic production hold constant. Thus, we are able to relate a percent change in water use (due to the addition of treated produced water) to a percent change in sector production.

The IMPLAN model is used to create a data set of economic benefits across economic sectors. Model runs are performed for differing target economic sectors (sector where water is added) and different assumed levels of growth. All outputs for economic benefits are at the county level and reported as changes in economic value by sector.

The IMPLAN model was run independently from PW-ESESim. IMPLAN was run under different economic sector assumptions and different levels of water availability to create a database of results that was then linked to PW-ESESim. This greatly simplifies future distribution as an open-sourced tool.

Due to the selection of a macroeconomic model such as IMPLAN, we are not able to conduct a micro level cost benefit analysis. Rather, the outputs of the IMPLAN model will provide economic benefits to the region demonstrating what could occur if the produced water is treated and made available to these economic sectors. The costs to treat and deliver the water are also calculated and influence the net economic benefit for projects of interest (Figure 3).

6. HUMAN AND ECOLOGICAL HEALTH MODEL

The screening level model used here is adopted from the Environmental Protection Agency's (EPA) E-FAST Model[5] used to support assessments of the potential exposures to new chemicals. The model generates estimates of chemical concentrations in surface waters (and groundwaters) and resultant dose rates to humans through ingestion, inhalation, and dermal exposure. The model can also be used to assess impacts to aquatic life and soils.

Here we are concerned with impacts on aquatic species due to stream augmentation with treated produced water; ingestion of fish from streams (Pecos) where treated produced water could be released; ingestion of Pecos water while swimming; inhalation of vaporized water from spray irrigation using treated produced water; and potential contamination of groundwater suppled for drinking. Note that there is no use of surface water in Eddy or Lea counties for drinking water.

This submodel will require inputs from other parts of PW-ESESim. Streamflow timeseries data will be input from the hydrology submodel. Similarly, produced water volumes and contaminant concentrations will be input from iDST. The dose rate calculations below are for individual contaminants of concern. As there are many potential contaminants remaining in the treated produced water, only a subset will be considered. Specifically, key indicator species will be identified that are representative of classes of contaminants of concern, e.g., metals, volatiles, radionuclides, salinity.

The model will be configured to estimate the baseline exposure (current dose rate using current water source, Table 6) and then the exposure when water source is changed to treated produced water (Table 7). Additional environmental concentrations will be compared to EPA's Regional Screening Level targets.

Table 6. Current average water quality parameter values for select constituents in southeastern NM. Also included are associated drinking water standards and concentration of concern levels.

Indicator (Category of Constituents)	surface water	groundwater	Concentration of Concern	Drinking Water MCL
Lead (Metals)	<1.1 ug/L	3.7 ug/L	15 ug/l	15 ug/L
Benzene (Volatile organic compounds)	Not detected	Not detected	0.46 ug/l	0.005 mg/L
ammonia-N (Nutrients)	0.15 mg/L	0.2 mg/L	Not defined	Not defined
nitrate-N (Nutrients)	1.2 mg/L	9.4 mg/L	3.2 mg/L	10 mg/L
Ra-126 and 128 (Radionuclides)	1.9 pCi/L	11.6 pCi/L	5 pCi/L	5 pCi/L
TDS (Salts)	4500 mg/L	1230 mg/L	500 mg/L	500 /L

6.1. Estimation of Potential Doses from Surface Water Bodies

The E-Fast Model estimates surface water concentrations in rivers and streams under four receiving stream flow conditions (1Q10 low flow, 7Q10 low flow, 30Q5 low flow, and harmonic mean flow) as recommended in the *Technical Support Document for Water Quality-based Toxics Control* (U.S. EPA, 1991).

[5] https://www.epa.gov/tsca-screening-tools/e-fast-exposure-and-fate-assessment-screening-tool-version-2014

Harmonic mean flows are used to generate estimates of chronic human exposure via fish ingestion. EPA recommends using the long-term harmonic mean to assess potential human health impacts because it provides a more conservative estimate than the arithmetic mean flow. The 30Q5 flows (lowest consecutive 30day flow during any five-year period) are used to generate estimates of acute human exposure via fish ingestion. To estimate potential acute and chronic inadvertent ingestion and aquatic life impacts, the model uses 1Q10 and 7Q10 flows, which are the lowest 1-day and the lowest consecutive 7-day average flows during any 10-year period, respectively. The stream data used are estimated flows at the downstream end of specific stream segments (reaches), and are presumed to include the discharge flow from any facility on that reach.

Stream related contamination will be limited to effects on the Pecos. Here we will use historical gage data above Brantley Reservoir (Table 8). Site-specific surface water concentrations are calculated from estimated arithmetic mean and 7Q10 stream flows. Harmonic mean, 30Q5, and 1Q10 flows are calculated from the 7Q10 flows and arithmetic mean flows. The units of flow are million liters per day (MLD). The estimated chemical concentrations are presented for each flow rate. The following are short definitions of the flows.

- **Harmonic Mean Flow ($SF_{harmonic}$)** — inverse mean of reciprocal daily arithmetic mean flow values. In other words, harmonic mean (H) is defined as $H = n/[(1/x_1) + (1/x_2) + ... + (1/x_n)]$ where x is a particular number in a group of measured values and n is the number of measurements in the series. These flows are used to generate estimates of chronic human exposures via drinking water and fish ingestion.
- **30Q5 Flow (SF_{30Q5})** — 30 consecutive days of lowest flow over a 5-year period. These flows are used to determine acute human exposures via drinking water.
- **7Q10 Flow (SF_{7Q10})** — 7 consecutive days of lowest flow over a 10-year period. These flows are used to calculate estimates of chronic surface water concentrations to compare with the constituents of concern (COCs) for aquatic life.
- **1Q10 Flow (SF_{1Q10})** — single day of lowest flow over a 10-year period. These flows are used to calculate estimates of acute surface water concentrations to compare with the COCs for aquatic life.
- **4Q3 Flow ($SF4_{Q3}$)** –4 consecutive days of lowest flow over a 3-year period. These flows are used by the State of New Mexico to calculate critical low flows.

The following equation is used to calculate surface water concentrations in free-flowing rivers and streams:

$$SWC = \frac{WWR * CF1}{SF * CF2} \quad (9)$$

where:
SWC = Surface water concentration (parts per billion (ppb) or µg/L)
WWR = Chemical release to wastewater (kg/day)
SF = Estimated flow of the receiving stream (MLD)
CF1 = Conversion factor (10^9 µg/kg)
CF2 = Conversion factor (10^6 L/day/MLD)

Table 7. Water quality values for treated produced water. Values in mg/L.

Treatment Level	Lead (metals)	Benzene (volatile organic compound)	ammonia-N (nutrient)	Nitrate-N (nutrient)	Ra-126/128 (radionuclide)	TDS (salt)
Drinking	0.015	0.005	2.0	10.0	4.0	500
Irrigation	0.005	0.005	2.0	10.0	4.0	1500
Clean Brine	0.015	0.005	2.0	10.0	4.0	25000

The amount of chemical released to the environment (e.g., produced water used for stream augmentation) are input values to this equation (output from iDST, Table 7). The conversion factor of 10^9 converts the chemical release from kg to µg. This value is then divided by the stream flow in MLD, which is converted to L/day (10^6 L/day/MLD). The results of this equation are chemical concentrations in units of µg/L. For very dilute aqueous solutions, the units of µg/L and ppb can be considered equivalent.

Surface water concentrations are calculated for four streamflow conditions (Equation 9). The equations used to estimate the harmonic mean, 30Q5, and 1Q10 flows from estimated arithmetic mean and 7Q10 flows (the arithmetic mean and 7Q10 are calculated directly from the modeled streamflow timeseries) also are presented below (Versar, 1992). The units for the arithmetic mean flow ($SF_{arithmetic}$) and the 7Q10 flow (SF_{7Q10}) used in these equations (Equations 10-12) are MLD. The factor 0.409 is used to convert MLD to units of cubic feet per second (cfs).

Harmonic mean stream flows are used to generate estimates of chronic human exposure via inadvertent ingestion and fish ingestion.

$$SF_{harmonic}(MLD) = 1.194 * \frac{\left(0.409\,\frac{cfs}{MLD} * SF_{arthmetic}\right)^{0.473} * \left(0.409\,\frac{cfs}{MLD} * SF_{7Q10}\right)^{0.552}}{0.409\,\frac{cfs}{MLD}} \qquad (10)$$

SF_{30Q5} (30 consecutive days of lowest flow over a 5-year period) stream flows are used to generate estimates of acute human exposures via inadvertent ingestion and fish ingestion.

$$SF_{30Q5}(MLD) = 1.782 * \frac{\left(0.409\,\frac{cfs}{MLD} * SF_{7Q10}\right)^{0.966}}{0.409\,\frac{cfs}{MLD}} \qquad (11)$$

SF_{7Q10} (7 consecutive days of lowest flow over a 10-year period) stream flows are used to generate estimates of exceedances of chronic COCs for aquatic life. SF_{1Q10} (single day of lowest flow over a 10-year period) stream flows are used to determine if there are acute ecological concerns.

$$SF_{1Q10}(MLD) = 0.843 * \frac{\left(0.409\,\frac{cfs}{MLD} * SF_{7Q10}\right)^{0.993}}{0.409\,\frac{cfs}{MLD}} \qquad (12)$$

Dose rates are then calculated using the concentrations calculated above (Equation 9). Here the concern is inadvertent ingestion of water while swimming by children and fish ingestion.

Table 8. Flow rates for Pecos River at Artesia (1960-2020). Values in Million Liters per Day

Statistic	Value (MLD)
Arithmetic Mean	404.6
Harmonic Mean	45.5
7Q10	4.4
30Q5	7.8
1Q10	3.7
4Q3	2.2

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from ingestion while swimming; calculated to represent chronic exposures to contaminated drinking water over a lifetime. These doses are generally used for cancer calculations.
- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in swimming water; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.
- **Potential Acute Dose Rate (ADR_{POT})** — from ingestion while swimming; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** — number of years a resident swims. Use model time horizon
- **Averaging Time (AT)** — period of time over which exposures are averaged. Use model time horizon
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Drinking Water Ingestion Rate (IR_{dw})** — used for calculating acute and chronic exposures.

The following equations are used to estimate how much of a given chemical a person will ingest while swimming. These equations convert an estimated surface water concentration to an exposure estimate. The surface water concentration (in µg/L) is multiplied by the estimated drinking water ingestion rate in liters per day, the number of release days per year, and exposure duration in years. This product is then divided by body weight (in kg) and averaging time to yield the exposure dose in mg/kg/day.

$$ADR_{POT} = \frac{SWC * IR_{dw} * RD * CF1}{BW * AT} \quad (13)$$

$$LADD_{POT} = \frac{SWC * IR_{dw} * ED * RD * CF1}{BW * AT * CF2} \quad (14)$$

$$LADC_{POT} = \frac{SWC * ED * RD * CF1}{AT * CF2} \quad (15)$$

where:
ADR_{POT} = Potential Acute Dose Rate (mg/kg/day)
$LADD_{POT}$ = Potential Lifetime Average Daily Dose (mg/kg/day)
$LADC_{POT}$ = Potential Lifetime Average Daily Concentration in drinking water (mg/L)
SWC = Surface water concentration (ppb or µg/L) use Equation 9
IR_{dw} = Swimming Ingestion rate (L/day) 0.0013 L/day (EPA Exposure Factors Handbook 2011)
RD = Release days (1 day for ADR_{POT}; 10 days/yr for $LADD_{POT}$ and $LADC_{POT}$)
BW = Body weight (kg) 32kg 6-11 yrs old (EPA Exposure Factors Handbook 2011)

ED = Exposure duration (use model time horizon)
AT = Averaging time (use model time horizon for $LADC_{POT}$ and $LADD_{POT}$; day for ADR_{POT})
CF1 = Conversion factor (10^{-3} mg/μg)
CF2 = Conversion factor (365 days/year)

The harmonic mean streamflow concentration is used to calculate the $LADD_{POT}$ and $LADC_{POT}$. The 30Q5 streamflow concentration is used to calculate the ADR_{POT}. This is consistent with EPA's OW guidance (U.S. EPA, 1991). The mean (central tendency) drinking water intake rate is used to calculate $LADD_{POT}$ and the high-end swimming ingestion rate is used to calculate ADR_{POT}.

6.2. Aquatic Health

The following metrics (as noted above) can be used to assess chronic and acute concentrations in surface water bodies for aquatic life:

- **7Q10 Flow (SF_{7Q10})** — 7 consecutive days of lowest flow over a 10-year period. These flows are used to calculate estimates of chronic surface water concentrations (Equation 9) to compare with the COCs for aquatic life[6].
- **1Q10 Flow (SF_{1Q10})** — single day of lowest flow over a 10-year period. These flows are used to calculate estimates of acute surface water concentrations (Equation 9) to compare with the COCs for aquatic life[7].

6.3. Fish Ingestion

The Fish Ingestion Information tab presents the exposure doses for individuals who ingest fish from streams and rivers that receive wastewater discharges containing the chemical of concern. The exposure types and exposure factors are defined below.

Exposure Types

- **Potential Lifetime Average Daily Dose ($LADD_{POT}$)** — from ingestion of fish tissue; calculated to represent chronic exposures to fish over a lifetime. These doses are generally used for cancer calculations.
- **Potential Lifetime Average Daily Concentration ($LADC_{POT}$)** — of the chemical of concern in ingested fish tissue; calculated to represent chronic lifetime concentrations. These concentrations are generally used for cancer calculations.
- **Potential Acute Dose Rate (ADR_{POT})** — from ingestion of fish tissue; normalized over a shorter time period (e.g., 1 day).

Exposure Factors

- **Exposure Duration (ED)** — length of time the fish consumer is exposed.
- **Averaging Time (AT)** — period of time over which exposures are averaged.
- **Body Weight (BW)** — mean body weight for the population being assessed.
- **Fish Ingestion Rate (IRfish)** — used for calculating acute and chronic exposures.

---

[6] https://www.epa.gov/wqc/national-recommended-water-quality-criteria-aquatic-life-criteria-table#table
[7] https://www.epa.gov/wqc/national-recommended-water-quality-criteria-aquatic-life-criteria-table#table

The following equations are used to estimate how much of a given chemical a person will ingest through eating fish. These equations convert an estimated surface water concentration to a fish ingestion exposure estimate. The distinction between acute and chronic fish ingestion is made on the basis of daily ingestion rate. The mean long-term fish ingestion rate is used to calculate chronic exposures and the mean serving size is used to calculate acute fish ingestion exposures for adults. This is in contrast to drinking water estimates, where the distinction between acute and chronic values is made on the basis of stream flows and on ingestion rates. The reason for this difference is that it takes time for chemical concentrations to accumulate in fish; therefore, the harmonic mean flow is used to calculate concentrations for both acute and chronic scenarios. It is not appropriate to use a very low streamflow value that occurs rarely as the basis for calculating a chemical residue in fish.

$$ADR_{POT} = \frac{SWC * BCF * IR_{fish} * RD * CF1}{BW * AT} \quad (16)$$

$$LADD_{POT} = \frac{SWC * BCF * IR_{fish} * ED * RD * CF1}{BW * AT * CF2} \quad (17)$$

$$LADC_{POT} = \frac{SWC * BCF * ED * RD * CF1}{AT * CF2} \quad (18)$$

where:
ADR_{POT} = Potential Acute Dose Rate (mg/kg/day)
$LADD_{POT}$ = Potential Lifetime Average Daily Dose (mg/kg/day)
$LADC_{POT}$ = Potential Lifetime Average Daily Concentration in fish tissue (mg/kg)
SWC = Surface water concentration (ppb or µg/L) from Equation 9
BCF = Estimate of chemical's bioconcentration potential (L/kg) see values for metals/radionuclides in Karlsson et al. 2002
IR_{fish} = Fish ingestion rate (kg/day) 12.3 g/day sport caught fish pg 10-33 (EPA Exposure Factors Handbook 2011)
RD = Release days (1 day for ADRPOT; days/yr for $LADD_{POT}$ and $LADC_{POT}$ based on produced water discharge schedule)
BW = Body weight (kg) use 80 kg (EPA Exposure Factors Handbook 2011)
ED = Exposure duration (use model time horizon)
AT = Averaging time (use model time horizon for $LADC_{POT}$ and $LADD_{POT}$; day for ADR_{POT})
CF1 = Conversion factor (10-3 mg/µg)
CF2 = Conversion factor (365 days/year)

Again, the harmonic mean streamflow concentration is used to calculate the LADDPOT and LADCPOT. The 30Q5 streamflow concentration is used to calculate the ADRPOT.

6.4. Estimation of Surface Water Exposure Concentrations in Lakes, Bays, Estuaries, and Oceans

No simple streamflow value represents dilution in these types of water bodies. To account for further dilution in the water body, dilution factors for the water body of interest are used. Measured dilution factors are typically between 1 (representing no dilution) and 200 and are based on National Pollutant Discharge Elimination System (NPDES) permits or regulatory policy. Here, to determine the dilution factors we will estimate dilution from a simple mass balance approach, balancing other local inflows, precipitation on the lake and evaporative losses. In this case dilution values are expected to be low.

The following equation to calculate surface water concentrations in still bodies such as bays, lakes, and estuaries:

$$SWC = \frac{WWR * CF1}{PF * CF2 * DF} \tag{19}$$

where:
SWC = Surface water concentration (ppb or µg/L)
WWR = Chemical release to wastewater (kg/day) from iDST
PF = Effluent flow of the discharging facility (MLD) based on produced water discharge schedule
DF = Acute or chronic dilution factor used for the water body (typically between 1 and 200) calculated by model (Brantley reservoir sub-model)
CF1 = Conversion factor (109 µg/kg)
CF2 = Conversion factor (106 L/day/MLD)

For the case of southeastern New Mexico there are a couple of reservoirs on the Pecos River (the only free flowing river in the region) – Brantley and Avalon reservoirs. However, these reservoirs are not expected to produce any dilution. Any rain on reservoir, local inflow and groundwater exchange are at best expected to be offset by reservoir evaporation. Given the screening nature of this tool, no dilution/enrichment of contamination by these lakes is estimated.

6.5. Estimation of Groundwater Exposure Concentrations and Doses from Releases to Landfills

A simple conservative method is used to estimate groundwater concentrations that may result from chemical releases due to land application of treated produced water.

Site-specific estimation of groundwater (drinking water) exposure from land application requires information on climate, soil, groundwater flow direction, and location of receptor drinking water wells. Because this level of information is commonly not available for screening-level estimates, a simple, conservative, generic method developed by EPA is used (U.S. EPA, 1987a). The only chemical specific parameter required is the organic carbon partition coefficient (log Koc), and it is assumed that a reliable value (measured or estimated) exists. It is also assumed that the substance does not degrade abiotically or biologically at a rate sufficient to significantly affect its potential to reach ground water.

This method is based on studies that modeled the groundwater concentrations that resulted from the land application of hypothetical nonvolatile compounds (i.e., Henry's law constant < 1E-05 atm-m3/mol) of varying soil sorption characteristics (i.e., log Koc values ranging from 0 to 4.5) in soil types with different organic carbon contents and groundwater hydraulic characteristics (U.S. EPA, 1996). The transport of the chemicals through the soil and groundwater was modeled using the SESOIL and AT123D models, respectively. The loading of chemicals in a 1-hectare landfill was assumed to be 1,000 kg/year for 10 years. The distance to groundwater was assumed to be 8 meters, and the depth of a drinking water well 200 meters from the edge of the landfill was set at 20 meters.

EPA used the results of these studies to develop a conservative method for predicting groundwater exposures from landfill disposals by assigning migration descriptors based on log Koc values and the maximum long-term (>70 year) average groundwater concentrations associated with those Koc values (Table 9).

Table 9. Log Koc Values and groundwater concentrations for different migrations

Mitgration Descriptor	Log Koc	Groundwater concentration (GCW) (mg/L per kg release)
Negligible – no migration		**None**
Negligible to slow	> 4.5	3.21E-6
Slow	<4.5 to 3.5	2.67E-5
Moderate	<3.5 to 2.5	5.95E-5
Rapid	<2.5	7.55E-5

Estimation of groundwater potential doses from releases to land applications is now considered. The following equations are used to estimate how much of a given chemical a person will ingest through groundwater (drinking water). These equations convert an annual chemical release and its estimated groundwater concentration (from the preceding section) to a drinking water exposure estimate. The release amount is multiplied by the groundwater concentration (per kg release), the removal rate (if any) of the chemical during treatment of the drinking water, the estimated drinking water ingestion rate, the exposure frequency, and the exposure duration. This product is then divided by body weight and averaging time to yield the exposure dose.

$$LADD_{POT} = \frac{LFR * GWC * \left(1 - \frac{DWT}{100}\right) * IR_{dw} * EF * ED}{BW * AT * CF1} \tag{20}$$

$$LADC_{POT} = \frac{LFR * GWC * \left(1 - \frac{DWT}{100}\right) * EF * ED}{AT * CF1} \tag{21}$$

where:
$LADD_{POT}$ = Potential Lifetime Average Daily Dose (mg/kg/day)
$LADC_{POT}$ = Potential Lifetime Average Daily Concentration in drinking water (mg/L)
LFR = Chemical release rate to landfill per site (kg/yr) see below
GWC = Groundwater concentration (mg/L per kg release/yr): see Table 10
IR_{dw} = Drinking water intake rate (L/day) Use 1.2 L/d (EPA Exposure Factors Handbook 2011)
BW = Body weight (kg) Use 80 kg (EPA Exposure Factors Handbook 2011)
DWT = Removal during drinking water treatment (percent) Assume zero at domestic wells, if near municipal well then include treatment
ED = Exposure duration (use model time horizon)
AT = Averaging time (use model time horizon for LADCPOT and LADDPOT)
EF = Exposure frequency (days/yr) Use 365 days/yr
CF1 = Conversion factor (365 days/yr)

Calculation of LFR is based on EPA's modeling assumptions of the mass of contaminant loaded in a "landfill" measuring 1 hectare. The following equation is used to calculate LFR from the volume and contaminant concentration given by the output of iDST:

$$LFR = \frac{Conc * Q * Area}{10000} \tag{22}$$

Where:
Conc = the contaminant concentration in the treated produced water (kg/m3) from iDST
Q = the volume of treated produced water (m3) from iDST
Area = the land area over which the treated produced water is spread (m2) defined by the scenario
The denominator is the number of meters in a hectare

Table 10. Mapping target analytes to their log Koc categories

Indicator (Category of Constituents)	log Koc category
Lead (Metals)	<3.5 to 2.5
Benzene (Volatile organic compounds)	<2.5
ammonia-N (Nutrients)	<2.5
nitrate-N (Nutrients)	<2.5
Ra-126 and 128 (Radionuclides)	<3.5 to 2.5
TDS (Salts)	<2.5

6.6. Inhalation

Inhalation exposure can result from breathing air that is contaminated with particulate matter (e.g., dust), vapors (e.g., volatile, or semi volatile contaminants), or aerosols. In this case, the primary concern is vaporized water from spray irrigation with treated produced water. Since Eddy county predominantly uses flood irrigation, inhalation only applies to irrigation in Lea county.

Estimating exposure from inhalation requires information on the concentrations of contaminants in the air and the timeframe over which inhalation exposure occurs. To calculate an inhaled dose, inhalation rates and receptor body weights might also be needed.

The methods used in developing noncancer inhalation dose-response values are discussed in more detail in the U.S. EPA report entitled Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry (USEPA, 1994).

The Superfund Program has also recently updated its approach for determining inhalation risk. It has eliminated the use of inhalation rates when evaluating exposure to air contaminants. This is described in *Risk Assessment Guidance for Superfund (Part F, Supplemental Guidance for Inhalation Risk Assessment)* (USEPA, 2009).

This updated methodology recommends that risk assessors use the concentration of the contaminant in air (Cair) as the exposure metric (e.g., mg/m3) instead of the intake of a contaminant in air based on inhalation rate and body weight (dose; e.g., mg/kg-day).

The adjusted air concentration (Cair-adj) may be estimated as shown below

$$C_{air-adj} = \frac{C_{air} * ET * \frac{day}{24\,hrs} * EF * ED}{AT} \tag{23}$$

Where:
Cair = Concentration of contaminant in air (mg/m3). Spray concentration is 0.019L/m3 (estimated from New & Fipps 2000 assuming a single sprayer emits 0.29 g/min with sprayers spaced 6/7 feet apart). To get air concentration multiply solute concentration by spray concentration
ET = Exposure time (hours/day) (24 hr/day) estimated from New & Fipps 2000
EF = Exposure frequency (days/year) (54 days/yr) estimated from New & Fipps 2000
ED = Exposure duration (use 1 yr)
AT = Averaging time (use 365 days)

6.7. Dermal Exposure

Dermal exposure is not considered. The inhalation pathway is expected to be more concerning for farm workers (vs. exposure working with wet soils). Dermal exposure from swimming is expected to be less of an issue relative to inadvertent ingestion.

6.8. Impact to Soils

Irrigation not only requires large water volumes, but also has stringent water quality criteria. Specifically, for produced water, parameters such as the sodium adsorption ratio are important criteria for ensuring that the water quality is sufficient to not damage crops. The sodium absorption ratio (SAR) is a calculation of the suitability for a water source for irrigation. The equation for the calculation is:

$$SAR = \frac{[Na^{+}]}{\sqrt{\frac{[Ca^{+2}] + [Mg^{+2}]}{2}}} \tag{24}$$

The concentrations of sodium (Na+), calcium (Ca+2), and magnesium (Mg+2) are in milliequivalents per liter. When irrigation water has high SAR values, above three, then much more control of salt accumulation is needed. Water with high SAR can be used if enough water is applied to wash the salts down below the root zone of the crops. The SAR and electrical conductivity (Ecw) of the water must be considered together to determine the probable effect of using the water for irrigation (Ayers and Westcot 1994). When the source water has a higher conductivity, then there is a greater potential for salt damage at lower SAR levels. Ecw normally is expressed as decisiemens per meter (dS/m), which is the same as siemens per centimeter (S/cm). Given the saline nature of produced water with high sodium content, the SAR and Ecw are both important parameters to consider before use.

Table 11 tabulates sodium, magnesium, and calcium levels in treated produced water. The conversion from EC to TDS is as follows:

$$EC(dS/m) = TDS(mg/L)/800 \tag{25}$$

Table 11. Water quality for calculating SAR. Values in mg/l.

Treatment Level	Calcium	Magnesium	Sodium
Drinking	50	0.0	0.0
Irrigation	0.0	0.0	0.0
Clean Brine	2500	400	35000

7. ENVIRONMENTAL JUSTICE

Although oil and gas production greatly contribute to southeastern New Mexico's economy, there are concerns about industrial impacts on local communities. First, hydraulic fracturing poses significant threat to environmental health and resource availability at the local level. Environmental exposures include water, air, and soil pollution, as well as hazards associated with stress, noise, vibration, and radioactivity (Gorski & Schwartz, 2019). Health outcomes associated with oil and gas development include increased prevalence of low birth weight, respiratory and dermatologic symptoms, high risk pregnancy, chronic headaches and fatigue, and several more negative health outcomes (Gorski & Schwartz, 2019). At a community scale, oil and gas production has impacted several aspects of the built, social, and economic environment (Gorski & Schwartz, 2019). Oil and gas development has also been shown to exacerbate income distribution, increasing economic disparity among community members (Berisha et al., 2020). At a larger scale, the combustion of fossil fuels contributes to the warming climate, perhaps the chief environmental concern among current and future generations (Masson-Delmotte et al., 2021).

The negative impacts associated with oil and gas development are especially important given the social and economic vulnerability of southeastern New Mexico. Namely, 15.8% of Lea County residents and 14.6% of Eddy county residents live below the poverty line, as compared to 12.3% nationally (Data USA, 2021a, 2021b). Additionally, the patient to doctor ratio in Lea County is 3,164: 1 and 3,047:1 in Eddy, as compared to 930:1 in the state (Data USA, 2021a). The majority of Lea County residents were also born outside of the United States (65.4%), nearly twice as much as the national averages (34%) (Data USA, 2021a). Social inequity in community planning and development are important considerations because communities at socioeconomic disadvantage are far more likely to bear the burden of industrial and agricultural contamination than their advantaged counterparts (Grineski et al., 2015; Hicks, 2020). Addressing this inequity is often termed environmental justice, which the Department of Energy defines as:

> *"Environmental justice is the fair treatment and meaningful involvement of all people, regardless of race, color, national origin, or income, with respect to the development, implementation, and enforcement of environmental laws, regulations, and policies. Fair treatment means that no population bears a disproportionate share of negative environmental consequences resulting from industrial, municipal, and commercial operations or from the execution of federal, state, and local laws; regulations; and policies. Meaningful involvement requires effective access to decision makers for all, and the ability in all communities to make informed decisions and take positive actions to produce environmental justice for themselves" (Department of Energy, 2021).*

Given the environmental risks of oil and gas development and the region's social and economic vulnerability, environmental justice is a critical consideration for ensuring sustainable use of resources in southeastern New Mexico.

7.1. Existing models

Two environmental justice models were consulted to inform creation of the environmental justice submodel.

The first was California Environmental Protection Agency's Environmental Justice Screening Tool (CalEnviroScreen 4.0), which combines multiple sources of pollutions and the characteristics that could increase the sensitivity of a population to pollution (August et al., 2021). Together, the parameters provide a relative evaluation of social vulnerability and environmental threat across the state of California. Parameters include environmental exposure (e.g., diesel particulate matter, drinking water contaminants, and pesticide use); pollution burden (e.g., groundwater threats, solid waste sites and facilities, and impaired water bodies); sensitive populations (e.g., asthma, cardiovascular disease, low birth weight prevalence); and socioeconomic factors (e.g., educational attainment, poverty, unemployment, and housing burden)(August et al., 2021).The CalEnviroScreen EJ metric ranges from 0-100 and represents the percentile ranking of each census tract, relative to others (August et al., 2021).

The second model consulted was the Washington State Department of Health's (WaDOH) Environmental Health Disparities tool (UW Department of Environmental & Occupational Health Sciences, 2019). Modeled after the CalEnviroScreen 4.0, WaDOH's tool uses similar social and environmental parameters and methodologies to create a ranked metric of environmental disparity. Unlike CalEnviroScreen, WaDOH's tool represents the value in deciles (rather than percentile) relative to all other census tracts in the state. The mapping tool also allows its users to explore important sociodemographic characteristics, such as racial distribution, age/sex distribution, and population counts for each tract of interest (UW Department of Environmental & Occupational Health Sciences, 2019). Lastly, WaDOH's tool uses overlay maps to display important place-based data, such as farmworker housing, childcare centers, and tribal land (UW Department of Environmental & Occupational Health Sciences, 2019).

7.2. Approach

Similar to the CalEPA and WaDOH tools, our proposed approach emphasizes environmental exposure as well as key socioeconomic and cultural factors. Under these general categories, the research team identified a series of indicators of environmental justice that would be particularly relevant to produced water management. Since the modeling activities do not explicitly capture changes in demographics or oil and gas infrastructure over time, we denote the indicators that are static (i.e., do not change) and dynamic (i.e., do change) across modeling scenarios.

Environmental Exposure:

- **Static**
    - **Proximity to oil and gas activity**: Research shows that proximity to O&G activity has been related to adverse birth outcomes such as low birth weight and small for gestational age births in rural communities (Tran et al., 2020). To capture these proximity measures, we calculated distances (using "as the crow flies" measure) between each township's centroid to the nearest O&G well (Figure 4).

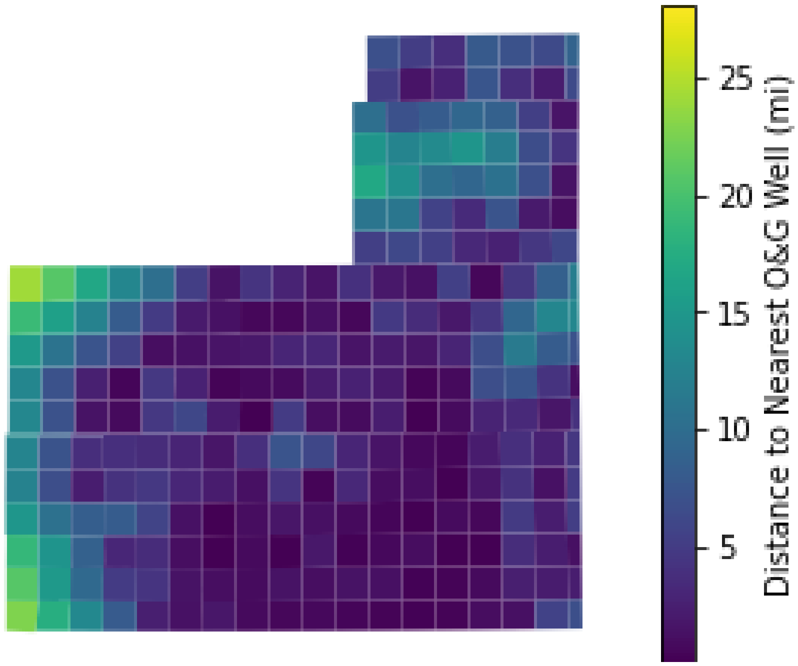

Figure 4. Proximity to O&G activity for Eddy and Lea County.

- **Proximity to PW disposal**: Research shows that produced water contains chemicals associated with adverse health effects, and can persist after wastewater treatment (Ferrar et al., 2013; Gross et al., 2013). So, the proximity of the salt water disposal wells to each township's centroid was calculated to capture this potential impact (Figure 5).

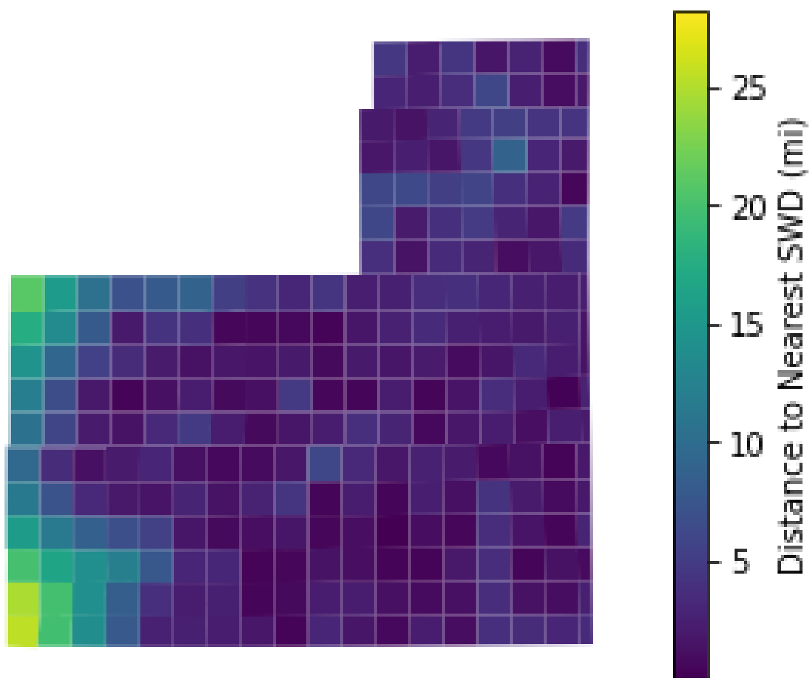

Figure 5. Proximity to nearest saltwater disposal well in Eddy and Lea County.

- **Dynamic**
  - **Proximity to heavy traffic**: Increased noise and light pollution has been shown to affect the psychological wellbeing of local residents (Fisher et al., 2018). Here we will develop a proxy with miles of truck traffic (see Section 3.5)
  - **Decreased water quantity**: Water use projections suggest variable impacts from water withdrawals, depending on water availability and competing demands at the local level (Nicot & Scanlon, 2012). Changes in this measure will be tracked by annual change in freshwater use in Lea and Eddy Counties (see Section 4.2).
  - **Impaired waters**: Discharged effluents, surface waters, and stream sediments from unconventional gas production often contain contaminants well over regulatory standards, which can threaten human health (Colborn et al., 2011). This metric will be tracked by noting changes in contaminant dose rates to the environment (Sections 6.1 and 6.5).

Socioeconomic:

- **Dynamic**
  - **Unemployment Rate**: Community members in oil and gas producing communities have debated the number of jobs created for local members of the community, and the impact on unemployment rate (Powers et al., 2015). Here we calculate the change in unemployment by simply subtracting added jobs due to a new produced water project from the unemployment rates in 2019.
  - **Poverty Rate**: Oil and gas development may increase income disparity in communities, which may negatively impact low-income families in the region (Berisha et al., 2020). Here we compare the income rate of added jobs vs. the average income of jobs in 2019.

Static parameters will be visualized as maps, while dynamic values are visualized over time, for each county, using model outputs from other sub-models.

8. PROOF-OF-CONCEPT: INTERACTIVE INTERFACE AND MODEL USE GUIDE

The following describes the basic layout for the PW-ESESim user interface and its use. The description is divided into input/scenario interface pages and the output interface.

First, there are a few general instructions to operating and navigating through the model. Once the user enters the model (pages beyond the initial splash page, see below), each page is fitted with basic model controls. At the far top right of each page is a picture of a home which will return to the home page or splash page from anywhere in the model. Next to the home page tab are a series of blue buttons that control the operations of the model; specifically:

- Double back arrows (left most button) resets the simulation. The simulation must be reset before making scenario selections or running a new simulation (more details below).
- The single forward arrow runs the model forward in time to the end of the simulation.
- The double vertical lines button pauses the simulation.
- The back arrow with two vertical lines steps through the simulation one year at a time.
- The question mark is currently not used.

Tabs for navigating through the various input and output pages of the model are organized along the left-hand side of each page. These are organized by Scenario or input pages (Map Interface, Project Setup, Produced Water Distributor) and Results pages (Beneficial Use, IMPLAN Results, Freshwater Summary, Human Ecological Summary, and Social Justice Summary). Simply click on the page that you desire to visit.

8.1. Input/Scenario Interface

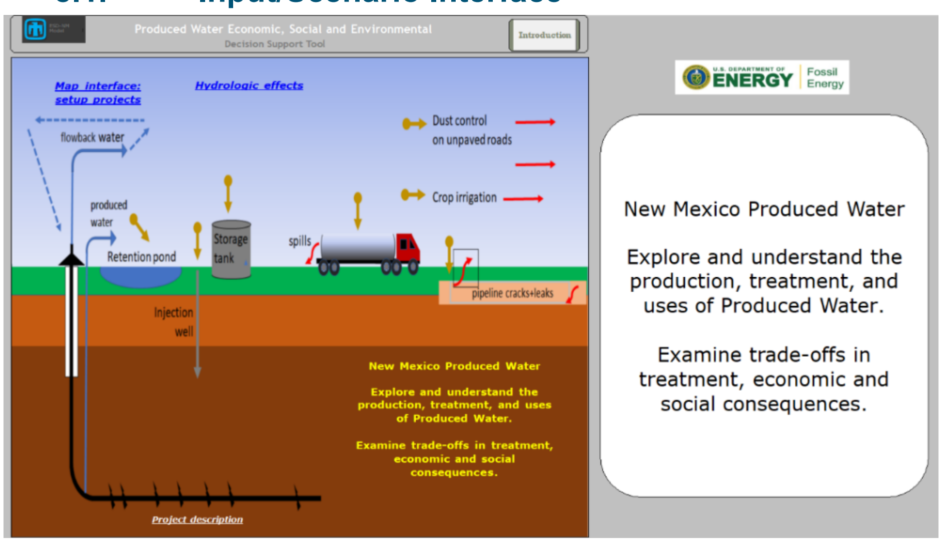

Figure 6. PW-ESESim opening or splash page.

When entering the model, the analyst is greeted by a splash page that depicts key aspects of the produced water cycle (Figure 6). Click on the “Introduction” or “Project Description” tab for background on the project and model. A click on the “Map Interface: Setup Projects” tab will direct the analyst to the first input interface page. This input interface allows the analyst to configure future scenarios for analysis. Configuration of a scenario first involves definition of a project’s location (the term project means a discrete development that will treat and use produced water). This is accomplished on the first input interface page (Map Interface page, Figure 7). A map of Lea and Eddy Counties is presented, while the analyst can choose among base maps by clicking on the associated radio button (oil wells, salt water disposal wells, produced water volume by township, and gas wells). The analyst can construct up to three projects for comparison for each model run. A project's location is designated by first clicking on the map in the desired location and then clicking on one of the tabs (project one; project two, project three) in the lower left. For reference the amount of water currently used in oil & gas, as well as the produced water generated in the selected township is referenced in the table in the upper right. Once project locations are selected the analyst moves to the next interface page by clicking on the "Go to Project Setup" arrow.

The analyst is directed to the "Project Setup Page" (Figure 8). Here projects are further defined in terms of the amount of water that is to be treated (not the desired product water) and the proposed use of the produced water. Treated water volumes are selected by clicking on the down arrow in the "Treatment Capacity" box. A dropdown menu will appear with three treated water volume options. Click on the desired option.

Next, click on the down arrow in the "Target Industry" box to define the purpose for the treated produced water. Again, several options are available—click on the desired option. Note that "Source Water Quality" is pre-defined based on the average TDS level for produced water generated in the township selected. Two other options representing brackish and saline water sources in the region are also provided. Click on either of these if a source water besides produced water is desired. Finally, the "End Use Water Quality" is automatically set based on the selected end use. Other treatment levels can be selected if desired. This process can be repeated for up to a total of three different projects per model run.

Additional input options are available by clicking on the "Produced Water Distributor" tab at the left (Figure 9). Here the analyst has additional scenario options pertaining to the rate at which produced water production grows, recycling of produced water in oil & gas development as well as how produced water is transported. First, the analyst can select the rate at which produced water production grows by adjusting the slider bar in the middle of the page (either positive or negative). Rates are adjusted separately for Eddy and Lea Counties, which are selected from the drop down box directly above the slider bar. Water used in oil & gas for drilling and stimulation currently is sourced from freshwater, brackish water, and recycled produced water. The analyst is allowed to change the mix of source water used in oil & gas development at a county level. For each county slider bars for each source water are provided. As one bar is adjusted the other two automatically adjust to balance use across the three options. The percent source water allocation is set to the current mix (Section 3. 2). To adjust one of the settings, first click on the green "Click here to Allow Input" and then click on the radio box next to the desired source water. Then slide the bar to adjust the source water to the desired level. Similarly, the analyst has the option to shift the mix in produced water transport (from the well to the treatment or disposal center) between trucking and pipeline (see Section 3.5). Adjustments are made in a similar fashion as described for oil & gas source water (see above).

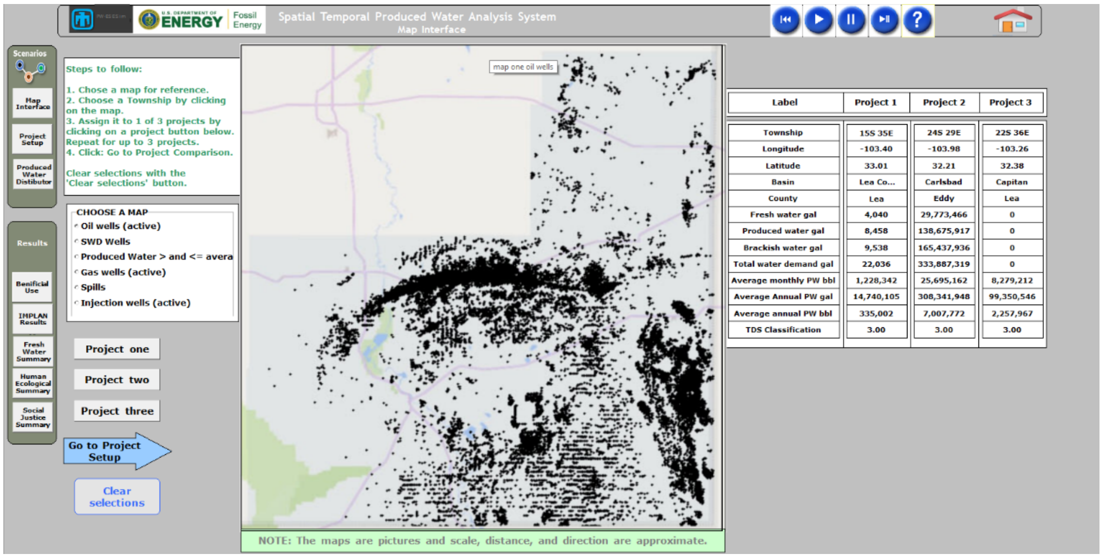

Figure 7. Input interface page (Map page) for designating project locations.

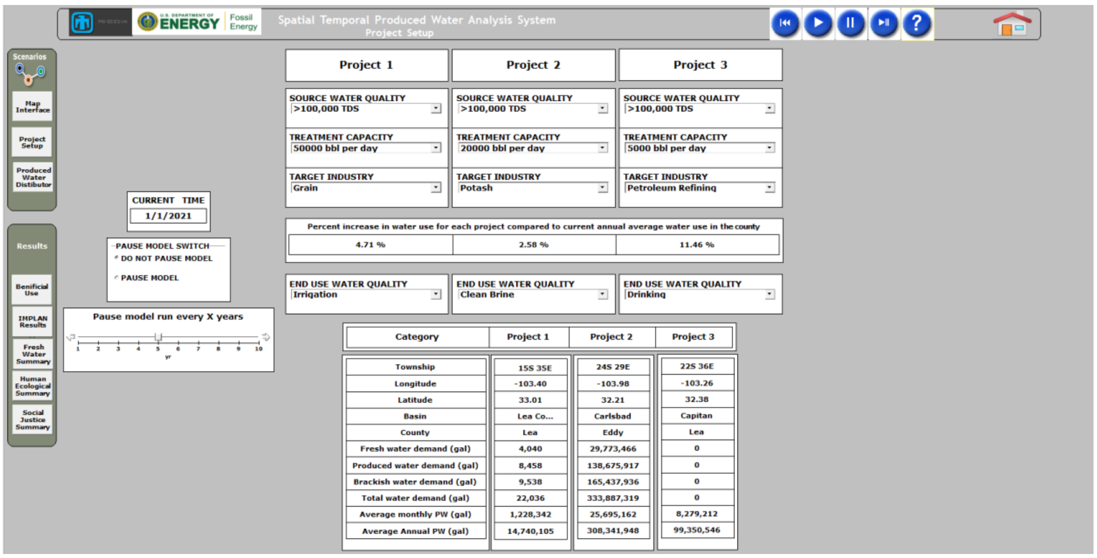

Figure 8. Project Setup page. Projects can be further defined in terms of desired treated water volumes and proposed use of the treated water on this page.

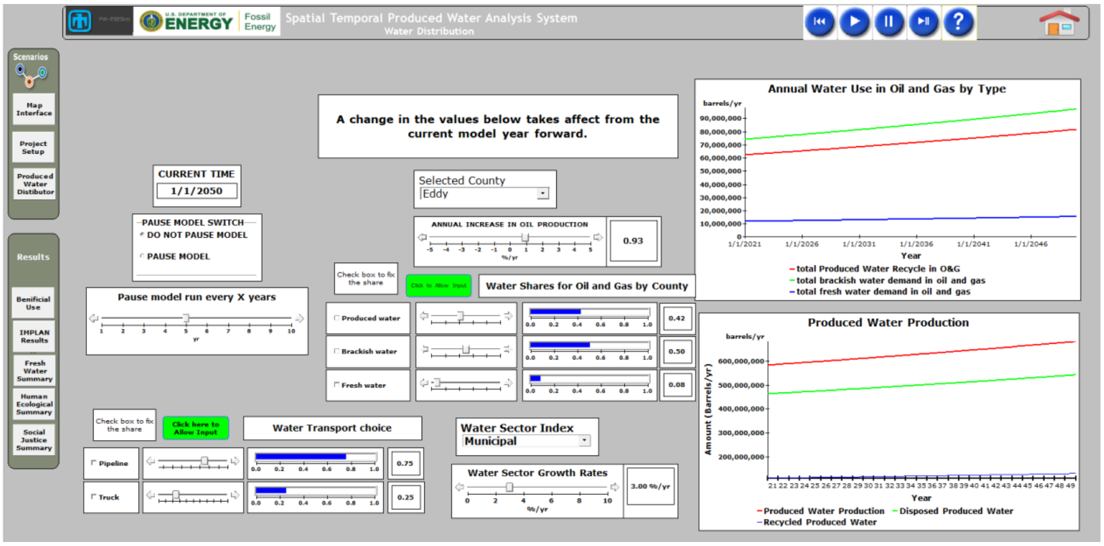

Figure 9. Input interface page. On this settings page, analysts can further define rates of produced water recycling and mix of mode of transportation.

8.2. Output Interface

The output interface is organized into individual pages for each of the key model sub-systems. Navigation between input and output pages is accomplished by clicking on the desired tab to the left side of each page. Output pages include:

- Beneficial Use,
- IMPLAN Results,
- Fresh Water Summary,
- Human Ecological Summary, and
- Social Justice Summary.

Note that on the "Produced Water Distributor Page" there are two output graphs. The top graph plots the mix of water sourced in oil and gas development from recycled produced water, brackish water, and freshwater over time. The second graph yields the total produced water generated, how much is disposed through deep-well injection and how much is recycled (in oil and gas or through other beneficial uses).

Beneficial Use: This page (Figure 10) reports results related to costs for the treatment and transport of produced water for the three projects selected above. Results are clearly organized according to the three produced water projects. At the top of the page the basic measures of each project are included. Below these results, reported general project information including required energy to treat the water, the produced water throughput, water recovery rate (the percent of throughput that is actually available for use, that is the final product water), and the recovered water in barrels/yr are reported. Then, below this are listed costs, including: 1) capital costs (facility and pipeline) and 2) variable costs (amortized capital costs assuming 15 years and 5% interest rate, and operating and maintenance costs). At the bottom of the leger are the summed variable costs, which are then inflated by various standard engineering continency costs as well as normalized treatment cost per barrel of product water are then provided. These costs are balanced by reduction in oil and gas operating costs due to reduced produced water disposal costs (e.g., product water times cost of disposal). The cost of disposal is set to a value agreed upon by local stakeholders but can be adjusted if desired (slider bar in upper part of page that is clearly marked). The bottom line gives the difference between the "Treatment Cost with Contingency" and "Cost Savings non-disposal of PW". On the left side of the page are results that don't depend on the project scenario, such as the cost of source water for oil and gas development (changes based on the mix of water used: brackish water $0.6 /barrel; Recycle PW $0.5/barrel; freshwater $1/barrel) as well as the cost to transport water by truck (current 25% of produced water generated).

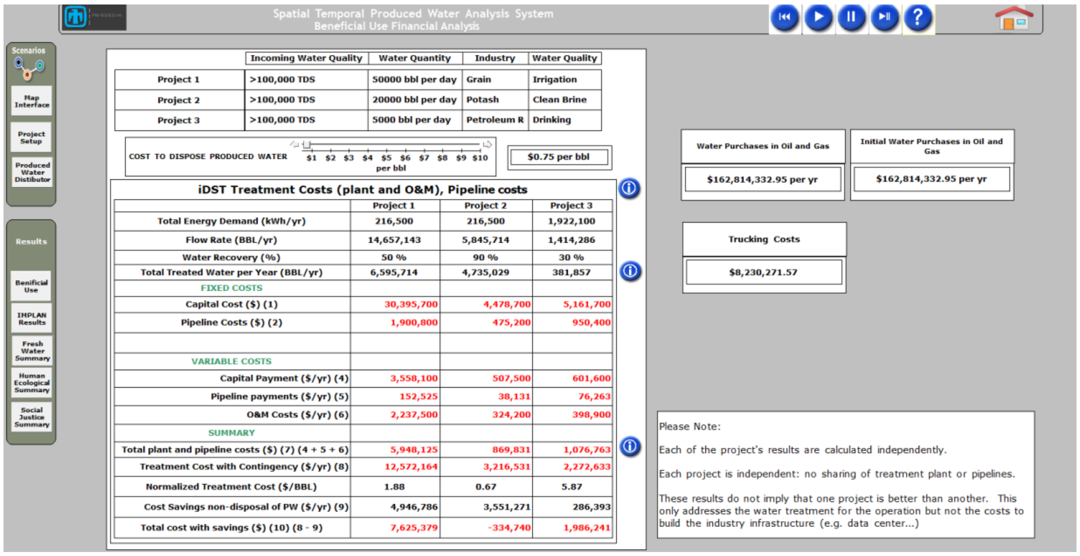

Figure 10. Beneficial Use page that provides results concerning the cost to build the three competing projects.

IMPLAN Results: This page reports the economic impacts resulting from the implementation of each of the three produced water projects. Again, the basic parameters of the three projects are provided at the top of the page. Below this, titled Economic Baseline, is the 2019 economic output for the county in which the project is sited. This includes employment, labor income, value added (secondary economic output) and total output. Below this, Economic Impact, is the same economic output but with implementation of the specified project. Finally, the Economic Change (i.e., the difference between the Economic Impact and Economic Baseline) is given (Figure 11). Specifically, this represents the growth in the local economy due to a given project. The evolution of these benefits and costs (from the Beneficial Use Page) over time are plotted to the right.

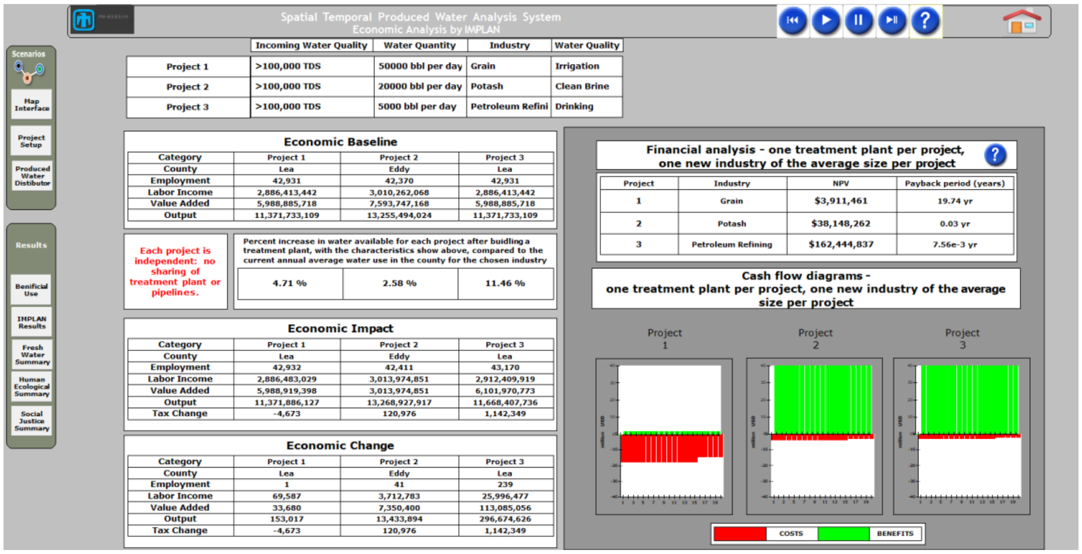

Figure 12. IMPLAN Results page that yields results on the economic impact, at the county level, resulting from the three competing projects.

Freshwater Summary: The "Freshwater Summary" page (Figure 12) captures changes in freshwater use resulting from changes in water demand across different water sectors. On the right-hand side of the page graphs are provided that plot changes in water use in the Municipal, Agricultural, and ICMP sectors according to their groundwater basin (or from the Pecos River). On the left-hand side a graph is provided that shows the change in water use by sector (i.e., aggregated over the six basins) relative to the 2019 rates. Note that results presented are for a single project. The analyst can choose the project to display by adjusting the "Select Project" slider to the desired project number (top center of page). The analyst can also adjust the annual growth rates for the different water use sectors by selecting the sector from the drop-down box and then sliding the bar to the desired rate (one must reset the model before these sliders can be adjusted). Recall that this region's water use is fully appropriated. That means that any increased demand for fresh water in oil & gas, municipal or ICMP will result in an equal decrease in Agricultural water use (assuming that farms are sold and water moved to these other uses).

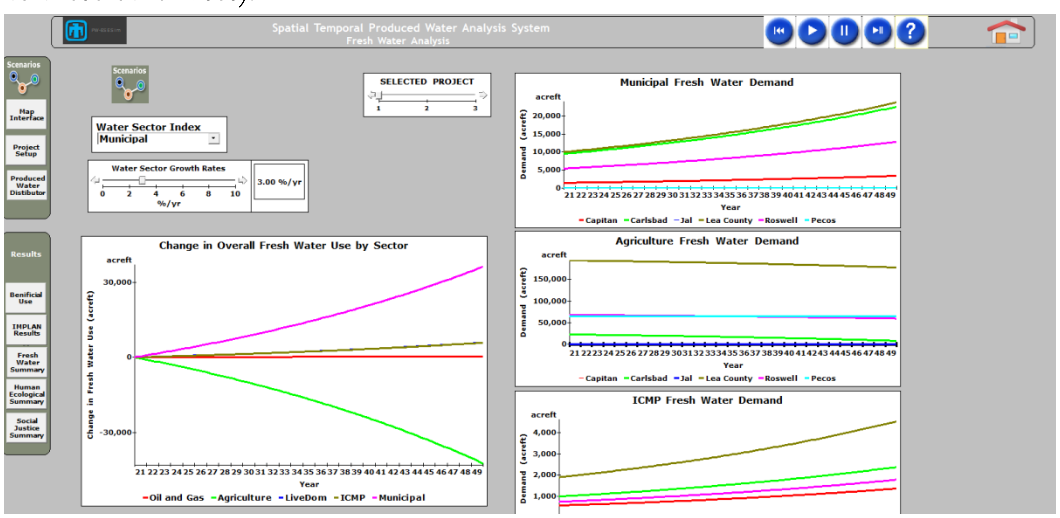

Figure 11. Freshwater Summary Page. This page yields results on impacts to freshwater use by basin and water use sector.

Human Ecological Summary: This page reports changes in water quality due to the reuse of treated produced water (Figure 13). Six different graphs are presented that describe changes to differing aspects of human and ecological health. Each graph displays results for six different indicator analytes (benzene, radium, ammonia, nitrate, TDS, and lead). For each analyte, the results of reusing treated produced water are compared to baseline concentrations in the Pecos River or local groundwater. Note that results are displayed for a single project at a time. The analyst can choose the project to display by adjusting the "Select Project" slider to the desired project number (top center of page). Baseline concentrations are always presented. However, results related to reuse of treated produced water are only displayed where applicable. Specifically, acute human exposure, chronic human exposure, acute fish exposure and chronic fish exposure only pertain to cases where the treated produced water is discharge to the Pecos river; hence, results are only displayed when "Pecos" is selected as the project "Target Industry". Groundwater dose and inhalation exposure apply only in cases where treated produced water is released directly to the environment for irrigation purposes.

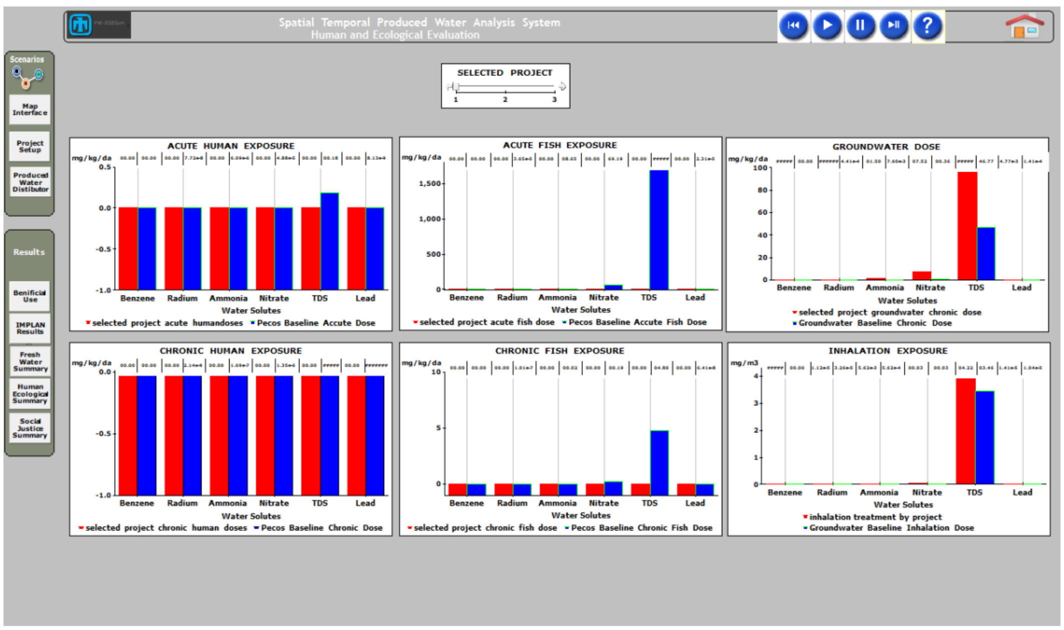

Figure 13. Human Ecological Summary page provides results on water and environmental quality impact due to the reuse of treated produced water.

Social Justice Summary: This page reports results related to societal impacts due to the reuse of treated produced water (Figure 14). The top graph addresses several different measures of social justice including job income, unemployment, farming acres (a measure of strength of the local culture), freshwater use, trucking miles for produced water and number of salt water disposal wells. In each case results are presented as a percent difference relative to conditions at the onset of the simulation. The lower graphs present changes in water quality relative to baseline concentrations. Again, these results are presented only for those cases where the treated water is released directly to surface water or groundwater sources. Results are displayed for a single project at a time. The analyst can choose the project to display by adjusting the "Select Project" slider to the desired project number (top center of page).

Figure 14. Social Justice Summary page provides results related to the societal impacts due to the reuse of treated produced water.

REFERENCES

Apergis, N. (2019). The impact of fracking activities on Oklahoma's housing prices: A panel cointegration analysis. *Energy Policy*, *128*, 94–101. https://doi.org/10.1016/j.enpol.2018.12.060

August, L., Bangia, K., Plummer, L., Prasad, S., Ranjbar, K., Slocombe, A., & Wieland, W. (2021). *CalEnviroScreen 4.0 Public Review Draft* (p. 201).

Ayers, R.S. and D.W. Westcot (1994). "Water quality for agriculture: The Infiltration Problem." Accessible online at: https://www.fao.org/3/T0234e/T0234E04.htm#ch3

Bauer, D., Philbrick, M., Vallario, B., Battey, H., Clement, Z., & Fields, F. (2014). The water-energy nexus: Challenges and opportunities. *US Department of Energy*.

Berisha, E., Chisadza, C., Clance, M., & Gupta, R. (2020). Income Inequality and Oil Resources: Panel Evidence from the United States. University of Pretoria, 22.

Blondes, M.S., Gans, K.D., Engle, Y.K. Kharaka, M.E. Reidy, V. Saraswathula, J.J. Thordsen, E.L. Rowan, E.A. Morrissey, U.S. Geological Survey National Produced Waters Geochemical Database v2.3 (PROVISIONAL), U.S. Geological Survey, 2017, https://energy.usgs.gov/EnvironmentalAspects/EnvironmentalAspectsofEnergyProductionandUse/ProducedWaters.aspx# 3822349-data.

Cather, D. Chen, Improving and Updating of the NM Produced Water Quality Database: Summary of New Mexico Produced Water Database and Analysis of Data Gaps, New Mexico Water Resources Research Institute and New Mexico Environment Department, 2016, https://nmwrri.nmsu.edu/wp-content/uploads/ProducedWater-Reports/Reports/Cather%20et%20al%202016%20-%20Improving%20and%20Updating%20of%20the%20NM%20Produced%20Water%20Quality%20Database%20Summary%20of%20NM%20PW%20Database%20and%20Analysis%20of%20Data%20Gaps.pdf.

Colborn, T., Kwiatkowski, C., Schultz, K., & Bachran, M. (2011). Natural Gas Operations from a Public Health Perspective. *Human and Ecological Risk Assessment: An International Journal*, *17*(5), 1039–1056. https://doi.org/10.1080/10807039.2011.605662

Data USA. (2021a). Eddy County Profile. Retrieved August 24, 2021, from https://datausa.io/profile/geo/eddy-county-nm

Danforth, C., McPartland, J., Blotevogel, J., Coleman, N., Devlin, D., Olsgard, M., ... & Saunders, N. (2019). Alternative management of oil and gas produced water requires more research on its hazards and risks. *Integrated environmental assessment and management*, *15*(5), 677-682.

Department of Energy. (2021). What Is Environmental Justice? Retrieved August 24, 2021, from https://www.energy.gov/lm/services/environmental-justice/what-environmental-justice

Dieter, C.A., Maupin, M.A., Caldwell, R.R., Harris, M.A., Ivahnenko, T.I., Lovelace, J.K., Barber, N.L., and Linsey, K.S., 2018, Estimated use of water in the United States in 2015: U.S. Geological Survey Circular 1441, 65 p., *https://doi.org/10.3133/cir1441*.

Dolan FC, Cath TY, Hogue TS. 2018. Assessing the feasibility of using produced water for irrigation in Colorado. Sci Total Environ 640–641, 619–628. https://doi.org/10.1016/j.scitotenv.2018.05.200

van Donkelaar, A., Martin, R. V., Brauer, M., Hsu, N. C., Kahn, R. A., Levy, R. C., et al. (2020). Global Annual PM2.5 Grids from MODIS, MISR and SeaWiFS Aerosol Optical Depth (AOD) with GWR, 1998-2016. Palisades, NY: NASA Socioeconomic Data and Applications Center (SEDAC). https://doi.org/10.7927/H4ZK5DQS. Accessed 1 April 2020. Palisades, NY: NASA Socioeconomic Data and Applications Center (SEDAC). Retrieved from https://doi.org/10.7927/H4ZK5DQS.

Ferrar, K. J., Michanowicz, D. R., Christen, C. L., Mulcahy, N., Malone, S. L., & Sharma, R. K. (2013). Assessment of Effluent Contaminants from Three Facilities Discharging Marcellus Shale Wastewater to Surface Waters in Pennsylvania. *Environmental Science & Technology*, *47*(7), 3472–3481. https://doi.org/10.1021/es301411q

Fisher, M. P., Mayer, A., Vollet, K., Hill, E. L., & Haynes, E. N. (2018). Psychosocial implications of unconventional natural gas development: Quality of life in Ohio's Guernsey and Noble Counties. *Journal of Environmental Psychology*, *55*, 90–98. https://doi.org/10.1016/j.jenvp.2017.12.008

Forrester, J. W., 1990. Principles of Systems. Productivity Press, Portland, Oregon.

Geza, M.; Ma, G.; Kim, H.; Cath, T.Y.; Xu, P. iDST: An integrated decision support tool for treatment and beneficial use of non-traditional water supplies – Part I. Methodology. Journal of Water Process Engineering 2018, 25, 236-246, doi:https://doi.org/10.1016/j.jwpe.2018.08.006.

Gorski, I., & Schwartz, B. S. (2019). Environmental Health Concerns From Unconventional Natural Gas Development. *Oxford Research Encyclopedia of Global Public Health*. https://doi.org/10.1093/acrefore/9780190632366.013.44

Grineski, S. E., Collins, T. W., & Aguilar, M. de L. R. (2015). Environmental injustice along the US–Mexico border: residential proximity to industrial parks in Tijuana, Mexico. *Environmental Research Letters*, *10*(9), 095012. https://doi.org/10.1088/1748-9326/10/9/095012

Gross, S. A., Avens, H. J., Banducci, A. M., Sahmel, J., Panko, J. M., & Tvermoes, B. E. (2013). Analysis of BTEX groundwater concentrations from surface spills associated with hydraulic fracturing operations. *Journal of the Air & Waste Management Association*, *63*(4), 424–432. https://doi.org/10.1080/10962247.2012.759166

Hicks, D. J. (2020). Census Demographics and Chlorpyrifos Use in California's Central Valley, 2011–15: A Distributional Environmental Justice Analysis. *International Journal of Environmental Research and Public Health*, *17*(7), 2593. https://doi.org/10.3390/ijerph17072593

Horn, A. D. Trading at Water Terminals. Shale Play Water Management. November - December 2019.

IMPLAN, 2021, IMPLAN: Economic Impact Analysis for Planning, at https://www.implan.com/

Ma, G. (2020). Permian Basin GIS Files. New Mexico State University.

Ma, G.; Geza, M.; Cath, T.Y.; Drewes, J.E.; Xu, P. iDST: An integrated decision support tool for treatment and beneficial use of non-traditional water supplies – Part II. Marcellus and Barnett Shale case studies. Journal of Water Process Engineering 2018, 25, 258-268, doi:https://doi.org/10.1016/j.jwpe.2018.08.007.

Masson-Delmotte, V., Zhai, P., Pirani, A., Conners, S. L., Pean, C., Berger, S., et al. (2021). Climate Change 2021: The Physical Science Basis. (Summary for Policymakers). IPCC. Retrieved from https://www.ipcc.ch/report/sixth-assessment-report-cycle/

National Energy Technology Laboratory (NETL). (2022) "Project PARETO - The Produced Water Optimization Initiative." https://www.project-pareto.org/

New Mexico Administrative Code (NMAC). 20.6.6 Title 20 Chapter 6 Part 4 Standards for Interstate and Intrastate Surface Waters.

New Mexico Oil Conservation Division, Produced Water Data Search, (2015) http://gotech.nmt.edu/gotech/Water/producedwater.aspx.

New, L., & Fipps, G. (2000). Center pivot irrigation. *Texas FARMER Collection*.

Nicot, J.-P., & Scanlon, B. R. (2012). Water Use for Shale-Gas Production in Texas, U.S. *Environmental Science & Technology*, *46*(6), 3580–3586. https://doi.org/10.1021/es204602t

O'Rourke, D., & Connolly, S. (2003). Just oil? The distribution of environmental and social impacts of oil production and consumption. *Annual Review of Environment and Resources*, *28*(1), 587-617.

Powers, M., Saberi, P., Pepino, R., Strupp, E., Bugos, E., & Cannuscio, C. C. (2015). Popular Epidemiology and "Fracking": Citizens' Concerns Regarding the Economic, Environmental, Health and Social Impacts of Unconventional Natural Gas Drilling Operations. *Journal of Community Health*, *40*(3), 534–541. https://doi.org/10.1007/s10900-014-9968-x

Scanlon, B. R., Reedy, R. C., Xu, P., Engle, M., Nicot, J. P., Yoxtheimer, D., ... & Ikonnikova, S. (2020). Can we beneficially reuse produced water from oil and gas extraction in the US?. *Science of The Total Environment*, *717*, 137085.

Sterman, J. D., 2000. Business Dynamics, Systems Thinking and Modeling for a Complex World. McGraw-Hill, Boston. 982 pp.

Tran, K. V., Casey, J. A., Cushing, L. J., & Morello-Frosch, R. (2020). Residential Proximity to Oil and Gas Development and Birth Outcomes in California: A Retrospective Cohort Study of 2006–2015 Births. *Environmental Health Perspectives*, *128*(6), 067001. https://doi.org/10.1289/EHP5842

USEPA. National Primary and Secondary Drinking Water Regulations. https://www.epa.gov/sdwa

USEPA: United States. Hazardous Site Control Division, United States. Environmental Protection Agency. Office of Solid Waste, & Emergency Response. (1996). *Soil Screening Guidance: User's Guide*. United States, Environmental Protection Agency, Office of Solid Waste and Emergency Response.

USEPA, 2020. Summary of Input on Oil and Gas Extraction Wastewater Management Practices Under the Clean Water Act, EPA 821-S19-001, at https://www.epa.gov/eg/summary-input-oil-and-gas-extraction-wastewater-management-practices-under-clean-water-act-final.

United States Department of Agriculture. NATURAL RESOURCES CONSERVATION SERVICE. Environment Technical Note No. MT-1 (Rev. 2). June 2011. https://www.nrcs.usda.gov/Internet/FSE_DOCUMENTS/nrcs144p2_051302.pdf

United States Department of Agriculture. Soil Conservation Service. Part 623 National Engineering Handbook. Chapter 2 Irrigation Water Requirements. Issued September 1993. https://www.wcc.nrcs.usda.gov/ftpref/wntsc/waterMgt/irrigation/NEH15/ch2.pdf

US Department of Housing and Urban Development. (2021). Location Affordability Index. Retrieved August 28, 2021, from https://www.hudexchange.info/programs/location-affordability-index/

UW Department of Environmental & Occupational Health Sciences. (2019). *Washington Environmental Health Disparities Map: Comparing environmental health risk factors across communities* (p. 44). Seattle, WA: UWDEOHS. Retrieved from https://deohs.washington.edu/sites/default/files/images/Washington_Environmental_Health_Disparities_Map.pdf

Veil, J., 2015. U.S. produced water volumes and management practices in 2012. Report Prepared for the Groundwater Protection Council, April 2015.