# **WaterTAP3 Documentation**

## version 0.0.2

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## **WaterTAP3 Documentation**

This is the documentation for the WaterTAP3 model.

### WaterTAP3 Overview

The Water Technoeconomic Assessment Pipe-Parity Platform (WaterTAP3) was developed under the National Alliance for Water Innovation (NAWI) to facilitate consistent technoeconomic assessments of desalination treatment trains. It is an analytically robust modeling tool that can be used to evaluate cost, energy, and environmental tradeoffs of water treatment technology across different water sources, sectors, and scales.

WaterTAP3 is publicly accessible and based on open-source models and data. The model is designed to be flexible and customizable to allow users to adapt or create new treatment trains and process models to assess different water treatment performance criteria.

Examples of WaterTAP3 applications include:

- Baselining the state of water treatment systems across key water-using economic sectors.
- Road-mapping critical technology development priorities to achieve pipe parity.
- Performing ongoing project evaluation for NAWI funded research.
- Conducting technoeconomic and life-cycle assessments of water technologies and systems across the water industry (in development).

### WaterTAP3 Installation

WaterTAP3 is still in development so is not listed in pip and must be accessed by cloning the current GitHub repo available at https://github.com/NREL/WaterTAP3.

- 1. Install the Anaconda distribution of Python:
  - https://www.anaconda.com/products/individual
- 2. Create new empty directory for WaterTAP3 installation:
  - e.g. this might be a folder called wt3 on your desktop
- 3. Open terminal and navigate to that directory:
  - e.g. cd ~/Desktop/wt3
- 4. Clone the repo:
  - In terminal, enter git clone https://github.com/NREL/WaterTAP3
  - For example, if you cloned the repo into ~/Desktop/wt3 , you will have a new directory ~/Desktop/wt3/WaterTAP3
  - All the necessary python files and data files will be downloaded into the WaterTAP3 directory.
- 5. Navigate to ~/WaterTAP3.
  - This directory contains the watertap3.yml file that is used to create the watertap3 Python environment.

- 6. Create the watertap3 Python environment.
  - In terminal, enter conda env create --file watertap3.yml
- 7. Activate the watertap3 Python environment.
  - In terminal, enter conda activate watertap3
- 8. Install the IDAES extensions to get solvers and function libraries:
  - In terminal enter idaes get-extensions
- 9. Navigate to ~/WaterTAP3/watertap3.
  - This directory contains the setup.py file that is used to install watertap3 as an editable Python package.
  - For example, if you cloned the repo into ~/Desktop/wt3, your working directory should now be ~/Desktop/wt3/WaterTAP3/watertap3.
  - This is also the directory that contains this documentation.
- 10. Install watertap3 as an editable Python package.
  - Must be in directory containing setup.py file
  - In terminal, enter python -m pip install -e .
  - NOTE: MUST INCLUDE THE PERIOD AT THE END OF THIS COMMAND
  - You should end up with new directory watertap3.egg-info in current directory
- 11. Start Jupyter Notebook app or Jupyter Lab app to run WaterTAP3.
  - For Jupyter Notebook jupyter notebook
  - For Jupyter Lab jupyter lab

## Running WaterTAP3

Running WaterTAP3 is done in a Jupyter notebook via sequential execution of three functions. All proper imports must be made before running WaterTAP3.:

```
from watertap3.utils import watertap_setup, get_case_study, run_model, run_watertap3
import pandas as pd
import numpy as np
```

Prior to executing these functions, you must define four variables to be used as inputs to the functions:

- case\_study A string that must match the name of your case study in all input files.
- scenario A string that must match the name of your scenario in all input files.
- desired\_recovery Targeted water recovery for your treatment train between 0-1 (default is 1).
- ro\_bounds A string that determines the maximum pressure limits for any reverse osmosis modules in your treatment train. Either 'seawater' for higher pressure limits (up to 85 bar) or 'other' for lower pressure limits (<25 bar). Default is 'seawater'.

The series of function executions are

- 1. m = watertap\_setup(case\_study=case\_study, scenario=scenario)
  - Reads in source water data and treatment train setup data.

```
2. m = get_case_study(m=m)
```

· Connects units and creates inlet, outlet, and waste ports.

```
3. m = run_watertap3(m, solver=solver, desired_recovery=desired_recovery, ro_bounds=ro_bounds)
```

• Runs WaterTAP3 model and saves results to ~/watertap3/watertap3/results/case\_studies.

This code block will execute all these steps.:

```
case_study = 'carlsbad'
scenario = 'baseline'
desired_recovery = 0.5
ro_bounds = 'seawater'
m = watertap_setup(case_study=case_study, scenario=scenario)
m = get_case_study(m=m)
m = run_watertap3(m, solver=solver, desired_recovery=desired_recovery, ro_bounds=ro_bounds)
```

### WaterTAP3 Cost Estimates

Cost estimations are represented at the unit process level (i.e. per treatment technology in the train) and aggregated to the system-level. Estimated costs include:

- Capital investment
- Annual operation and maintenance
  - Fixed (labor, maintenance)
  - Variable (energy, chemical)

## WaterTAP3 Outputs

The key performance metrics from WaterTAP3 currently include:

- Levelized Cost of Water (LCOW): cost per unit of treated water
- Energy intensity: direct energy consumption per unit of treated water
- Water recovery: the percentage of water recovered for a beneficial use
- Constituent removal: the percentage of constituent mass removed from the source water

Other outputs in development include:

- Extent of alternative water and energy resources
- Life-cycle assessment of environmental impacts (e.g. greenhouse gas emissions, total water intensity)
- · System resiliency and security

## WaterTAP3 Impacts

The objective of WaterTAP3 is to become a standard tool to evaluate water treatment system performance across key metrics used to promote and assess pipe-parity for a range of users including industry and academia. The results from WaterTAP3 can help identify trade-offs among the different performance metrics and enable users to asses how particular technologies affect pipe-parity metrics and how improvements in one metric can affect others across a range of source water conditions and technology performance parameters.

The flexibility and comprehensive scope of WaterTAP3 make it a useful tool for industry-wide technoeconomic analyses, promoting better informed water investment decisions and technology development. The tool can be used by policymakers, planners, and others without extensive analytical experience through the publicly available graphical user interface (under development).

## WaterTAP3 Framework

WaterTAP3 simulates steady-state water treatment train performance and costs including flow and constituent mass balance across unit processes, based on source water conditions, configurations of treatment technologies, and system-level techno-economic assumptions. Capital costs, operating costs, and unit performance are estimated for both individual treatment processes and the system as a whole. Users can perform new analysis either by selecting an existing train from the treatment train library or connecting any number of unit processes together in a custom configuration.

The model contains various technical and cost parameter options for several treatment technology models and a library of influent water quality characteristics for a variety of source waters. Users can customize water quality parameters to evaluate technology performance for their unique conditions. The model can be used for different assessment needs, including process simulation, optimization, uncertainty analysis, and sensitivity analysis.

### **Model Structure**

WaterTAP3 is implemented in Python using the Institute for the Design of Advanced Energy Systems (IDAES) which is itself based on the Python optimization and modeling package package Pyomo. Though initially developed for the research of innovative energy processes, at its core the IDAES framework is used to track material and energy flows through complex systems, making it useful for tracking water flows, chemical concentrations, and other parameters (e.g. pressure, temperature) through a treatment train.

Every WaterTAP3 model  $\mathfrak m$  is instantiated as a Pyomo <code>ConcreteModel()</code> object upon which an IDAES <code>FlowsheetBlock()</code> is placed to facilitate water and material transfers through each unit process in the WaterTAP3 model. Each unit model in WaterTAP3 is an instance of the <code>WT3UnitProcess()</code> class, which has properties inherited from the IDAES <code>UnitModelBlockData()</code> class. Connections between unit models are represented by the IDAES <code>Arc()</code> class.

Much like actual treatment technologies, material and energy exchanges in WaterTAP3 are facilitated by "ports" assigned to each unit process. Each water source and unit process is added as an attribute to the flowsheet and by default are given one inlet port, one outlet port, and one waste port. Additional inlet and outlet ports are added dynamically based on the input file (treatment\_train\_setup.csv - discussed in the Treatment Train Setup section of this documentation). Flow and mass balance is achieved across each unit process based on water recovery values and constituent removal factors.

## **Data Input for WaterTAP3**

This section describes the data input .csv files contained in the data folder located in the watertap3 directory. Many of these files applications and uses in WaterTAP3 are fully discussed in other sections, but their headings and a basic descriptions are presented here.

### basic unit.csv

This .csv file provides the inputs for unit process models that are initiated with the basic\_unit module (fully discussed in the unit process section of this document).

Capital costs for basic units based on water or mass flow are calculated with the general form:

$$C_{basic} = Bf^{x}$$

The ratio of the unit water flow (or mass flow) to the basis water flow (or mass flow) is the scaling factor *f* used to scale the unit costs to the basis costs:

$$f = \frac{Q_{in}}{Q_{basis}}$$

More detail is available in the Basic Unit unit process documentation.

The headings for basic\_unit.csv are:

- unit\_process: The unit process name provided by user input.
- flow\_basis: The flow basis for the unit process costing curve. This is either volume [m3/hr] or mass [kg/hr] based.
- cap\_basis: The capital basis for the unit process costing curve.
- **cap\_exp**: The exponent *x* for the costing curve.
- elect: Electricity intensity for the unit [kWh/m3]. This value is fixed.
- year: Costing year for the unit.
- kind: Indicates whether the unit is based on volumetric or mass flow.

### case\_study\_basis.csv

This .csv contains the foundational technoeconomic assumptions for the entire treatment train. This input is also discussed in the Financial Basis Inputs section of this documentation and inputs from this data file are used throughout the Financials section of this documentation.

The file is arranged into the following columns:

- case\_study: The treatment facility name.
- scenario: The name of the scenario that the TEA values correspond with
- value: The number or name of the variable of interest
- reference: The name of the project that is using the model
- variable: The name of the variable of interest
  - analysis\_year. The first year of the plant is/was in operation
  - *location\_basis*: The country or U.S. state where the plant is located. Used for assigning the electricity cost [\$/kwh]. Electricity costs are provided in the data folder.
  - plant\_life\_yrs: The initial design basis for plant-life and used for life cycle analysis calculations. The default plant-life is 20 years.

- land\_cost\_percent: The assumed cost of land as a percentage of total fixed capital investment. This is
  a part of the total capital investment.
- working\_capital\_percent: The assumed cost of working capital as a percentage of total fixed capital investment. This is a part of the total capital investment.
- salaries\_percent: The assumed cost of salaries as a percentage of total fixed capital investment. This
  is a part of the fixed operating costs.
- employee\_benefits\_percent: The assumed cost of employee benefits as a percentage of total salary cost. This is a part of the fixed operating costs.
- maintenance\_cost\_percent: The assumed cost of maintenance as a percentage of total fixed capital investment. This is a part of the fixed operating costs.
- laboratory\_fees\_percent: The assumed cost of laboratory fees as a percentage of total fixed capital investment. This is a part of the fixed operating costs.
- insurance\_and\_taxes\_percent: The assumed cost of insurance and taxes as a percentage of total fixed capital investment. This is a part of the fixed operating costs.
- default\_cap\_scaling\_exp: The typical value for economy-of-scale for capital equipment. This is a part of the total and fixed capital investment.
- default\_opex\_scaling\_exp: The typical value for economy-of-scale for fixed plant costs. This is a part of the fixed operating costs.
- cap\_by\_equity: The percent of the capital that is financed by equity rather than debt. This is a part of the capital recovery factor and LCOW calculations.
- debt\_interest\_rate: The rate for loan financing of capital. This is a part of the capital recovery factor and LCOW calculations.
- exp\_return\_on\_equity: The expected return, interest rate, or cost of capital associated with the portion
  of capital financed with equity.
- default\_tpec\_multiplier. The Total Purchased Equipment Cost (TPEC) to fixed capital investment. This is a part of the total and fixed capital investment calculations.
- default\_tic\_multiplier. The Total Installed Cost (TIC) to fixed capital investment. This is a part of the total and fixed capital investment calculations.

#### case\_study\_water\_sources.csv

Source water information is required to run the model. It can be selected from a list of pre-existing case studies or entered manually using Jupyter Notebook or the input data tables in this .csv file. There is no limit on the number of source water nodes for the model and the treatment train design section details how to connect source waters to the treatment train. Water flow rates (volumetric) and any constituent information required to calculate a unit process performance or cost must exist in the source water information.

The source water input dataset is arranged into the following columns:

- case\_study: The treatment facility name.
- scenario: The name of the scenario that the values correspond with, otherwise the default value will be used.
- water\_type: The type/source of the water. This is where the intake unit water\_type names must match the train
  input water\_type process parameter in the treatment train design.
- variable: The name of the constituent or property of interest, such as 'flow' (required) or 'tds'.
- value: The number of the variable of interest
- unit: The units used for the constituent, such as kg/m3 (constituent concentration)
- reference: The name of the project.

### catalyst\_chemicals.csv

This .csv contains the price data used to calculate chemical and catalyst costs. WaterTAP3 uses the unit per volume (typically a dose as kg/m3) and the price in this .csv to calculate costs. More information on how this file is used is in the Variable Operating Costs section of this documentation.

#### The columns are:

- Material: Name of the material, catalyst, or chemical used in the unit process. Note that when user input is required for a catalyst or chemical (e.g. in the Chlorination unit module), the input must match *exactly* with the name in this column.
- Price\_Units: The units associated with the Price column. Typically \$/kg.
- Price: The price per unit used to calculate costs.
- Price\_Year: The pricing year. Used to calculate a chemical index factor.
- Purity: The purity of the chemical used for pricing.

### chemical\_addition.csv

This .csv contains data used to construct costing curves for different chemicals in the chemical\_addition unit module. A user could add an entry to this .csv if there is a chemical that is not represented here if they have a value for each column. More information on how this unit works is provided in the chemical addition unit module.

#### The columns are:

- **chem\_name**: Name of the material, catalyst, or chemical used in the unit process. Note that the chemical name provided by user input must match *exactly* with the entry in this column.
- base: The costing basis for the chemical addition used to construct the costing curve.
- exp: The exponent for the chemical addition used to construct the costing curve.
- ratio: The ratio of the chemical in the solution used in the source costing data.
- density: The density [kg/m3] of the chemical in the solution used in the source costing data.

#### chlorine\_dose\_cost.csv

This .csv contains costing data used in the chlorination unit module. This data is used as the basis to calculate the capital costs for chlorination based on unit flow and chlorine dose. The data in this file comes from the User's Manual for Integrated Treatment Train Toolbox - Potable Reuse (IT3PR) Version 2.0.

#### The columns are:

- Cost: The cost associated with the dose and flow [\$1000].
- Dose: The chlorine dose used for costing [mg/L].
- Flow\_mgd: The flow used for costing [MGD].

### constituent\_removal.csv

This .csv contains default and case specific constituent removal factors. More information on how these factors are used is discussed in the Constituent Removal section of this documentation.

#### The columns are:

- case\_study: The treatment facility name.
- scenario: The name of the scenario associated with the removal fraction.
- units: The units used for the constituent, such as kg/m3 (constituent concentration).
- unit\_process: The unit process with the associated removal.
- value: The fraction or percent of the constituent in the source water that will be removed.
- constituent: The constituent being removed as named in the model.

- calculation\_type: How the model will handle the values when the unit process changes the constituent level, ultraviolet transmittance, or pH.
  - fractional\_constituent\_removal: fractional removal
  - absolute\_value: percent removal for ultraviolet transmittance
  - delta\_constituent\_or\_property: when the pH is changed
- reference: The name of the project that is using the model.
- data\_reference: The source of the data values and how values were calculated. Not used in the model but presented for user reference.
- constituent\_longform: The longform name of the constituent. Not used in the model but presented for user reference.

#### cost\_curves.csv

This .csv contains summary outputs for different EPA model runs at different flow rates. The EPA models can be found at https://www.epa.gov/sdwa/drinking-water-treatment-technology-unit-cost-models

Outputs from these EPA models is used for the following WaterTAP3 unit modules:

- Cation Exchange
- Anion Exchange
- fixed bed pressure vessel unit
- Fixed Bed Pressure Vessel
- multi\_stage\_bubble\_aeration\_unit
- packed\_tower\_aeration\_unit
- GAC Pressure Vessel
- GAC Gravity

Further explanation of how this data is used in those unit models is provided in the documentation for each respective unit. In short, data from the flow\_in, cap\_total, and electricity\_intensity columns are used to construct cost curves as a function of flow [m3/hr] to determine capital costs and electricity intensity for each of these units.

The columns are:

- unit\_process: The name of the WaterTAP3 unit module.
- flow\_in: The flow [m3/hr] used to construct the cost curve.
- cap\_total: Summation of the direct, indirect, and add-on costs from the EPA model runs.
- electricity\_intensity: Electricity intensity data from EPA model runs.
- tds\_in: Used by the Cation Exchange and Anion Exchange unit model to select the proper cost curve to use for the given TDS into the unit. If the unit does not have an entry in this column, it is not a function of this variable.
- num\_stage: Used by the Multi-Stage Bubble Aeration unit model to select the proper cost curve based on the number of stages in the unit (determined from user input). If the unit does not have an entry in this column, it is not a function of this variable.
- radon\_rem: Used by the Packed Tower Aeration unit model to determine the proper cost curve based on the target amount of radon removal (determined from user input). If the unit does not have an entry in this column, it is not a function of this variable.
- ebct: Used by the GAC Gravity and GAC Pressure Vessel unit models to determine the proper cost curve to used based on the EBCT (determined from user input). If the unit does not have an entry in this column, it is not a function of this variable.

The columns to the right of ebct are materials names specific to each unit model that uses this .csv. If there is no entry for the unit model under one of these columns, that unit model does not use that chemical. For example, the Cation Exchange unit model uses Ion\_Exchange\_Resin, but does not use Acetic\_Acid. The values in each of these columns correspond to a dose for that chemical. WaterTAP3 takes the average of the entire column as the dose for that material or chemical which is then used to calculate chemical costs.

## electricity\_costs.csv

This .csv contains location specific electricity costs used to determine the electricity costs for the model.

The columns are:

- location: The location for the case study determined from the case\_study\_basis.csv.
- cost: The \$/kWh price of electricity in that location.

### plant\_cost\_indices.csv

This .csv contains costing indices data.

There are four types of cost indices applied in WaterTAP3 – Capital, Catalysts and Chemicals, Labor and Consumer Price Index. WaterTAP3 calculates each of these indices for 1990-2050. These factors are used to help account for the time-value of investments and are used in the capital and operating cost calculations.

- Year: The year for the costing index.
- Capital Index: The capital index for the given year.
- CatChem\_Index: The catalyst and chemical index for the given year.
- Labor\_Index: The labor index for the given year.
- CPI\_Index: The consumer price index (CPI) for the given year.

Further information on how these values are used in WaterTAP3 is available in the Costing Indices and Factors section of this documentation.

### treatment\_train\_setup.csv

This .csv is how treatment trains are setup in WaterTAP3. Please refer to the Treatment Train Setup section of this document for an in-depth description of this file and how it is used to create custom treatment trains in WaterTAP3.

### uv\_cost\_interp.csv

Contains interpolated data from User's Manual for Integrated Treatment Train Toolbox - Potable Reuse (IT3PR) Version 2.0 used to calculate the capital costs of a UV/AOP system as a function of flow, dose, and UV transmittance.

The columns are:

- dose: The UV dose [mJ/cm2] (from user input) used to determine capital costs.
- flow: The flow [MGD] used to determine capital costs.
- uvt: The UV Transmittance (from user input) used to determine capital costs.
- cost: The cost [\$1000] as a function of dose, flow, and UVT.

More information in the UV + AOP model documentation.

#### water\_recovery.csv

This .csv contains fractions of water recovery for each unit in WaterTAP3. More information on how this data is used in WaterTAP3 is available in the Water Recovery section of this documentation.

The columns are:

• case\_study: The treatment facility name or default

### Data Input for WaterTAP3

- scenario: The name of the scenario that the values correspond with
- unit\_process: The name of the unit process corresponding to the recovery value.
- recovery: How much water is recovered by each unit process (%)
- reference: The source of the recovery data

## **Model Output for WaterTAP3**

This section describes the model results files and directory.

## **Directory Structure**

Directory Structure for baseline analyses:

```
Source Water/
 -- baseline/
       -- Case study_baseline.csv (Case study specific baseline full results. Multiple file
       -- Source water_baseline.csv (Combined case study baseline full results)
       -- Summary table_Source Water_baseline.csv (Key baseline results for source water)
       -- figures/ (Treatment category level results)
             -- Annual O&M Costs_baseline
             -- Electricity Intensity System Treated_baseline
             -- LCOW_Cost_Category
             -- Total Capital Investment (TCI)_baseline
            -- Treatment Category LCOW_baseline
       -- csvs/
           -- CSV files used to create figures in "figures" directory
        -- by_unit/
            | -- CSV and figures for key cost results by unit process within the treatment t
  -- baseline_and_whatifs/
      | -- Same structure as baseline folder but includes what-if scenarios
    sensitivities/
       -- Figure of LCOW ($/m3), electricity intensity (kwh/m3) and water recovery (%) for
       -- CSV of results used to create the figure.
```

### Results File

Flow rates, constituent levels, and key cost attributes are reported for each unit process in a treatment train. System-level metrics including aggregate costs, energy use, recovery rate, and Levelized Cost of Water (LCOW) are also included.

The results table is arranged into the following columns (bold):

Case Study: The treatment facility name

Metric: The category for what is being measured. Examples are:

- Electricity
- Cost
- Annual Cost
- Water Flow
- Inlet Constituent Density
- Outlet Constituent Density
- Waste Constituent Density
- Inlet Constituent Total Mass
- Outlet Constituent Total Mass
- Waste Constituent Total Mass

Scenario: The name of the scenario that the values correspond with ex. baseline or what-if scenarios

Unit Process Name: The unit process name or "System".

**Unit**: The units used for the results value. Examples are: • Electricity intensity: kWh/m3 • Total costs: \$MM • Annual costs: \$MM/yr • Flow rates: m3/s • Water constituents: kg, kg/m3

**Value**: The outlet result at the end of a unit process or the entire treatment train.

Variable: The variable name that corresponds to the value. Examples are:

- Electricity Intensity [kWh/m3]
- Total Capital Investment (TCI) [\$MM]
- Catalysts and Chemicals [\$MM/yr]
- Electricity [\$MM/yr]
- Other Variable Operating [\$MM/yr]
- Fixed Operation [\$MM/yr]
- Annual O&M Costs [\$MM/yr]
- Inlet Water [m3/s]
- Outlet Water [m3/s]
- Waste Water [m3/s]
- Names of constituents in the source water [kg] and [kg/m3]

The results for an entire treatment train are: • System Total Capital Investment (TCI) [\$MM] • System Catalysts and Chemicals [\$MM] • System Electricity [\$MM] • System Catalysts and Chemicals [\$MM/yr] • System Electricity [\$MM/yr] • System Total Operating Cost [\$MM/yr] • System LCOW [\$/m3] • Electricity Intensity [kWh/m3] • Water Recovery [%]

Unit kind: Intake, treatment process, or end-use as represented in the model

**Treatment Category**: Influent Storage and Pumping, Pre-treatment, Principal treatment, Product Storage, Product Distribution, Waste Treatment and Valorization, Waste Product Storage and Disposal, Post-treatment

## **Source Water**

data/case\_study\_water\_sources.csv

Source water information is required to run the model. It can be selected from a list of pre-existing case studies or entered manually using Jupyter Notebook or the input data tables in the data folder. There is no limit on the number of source water nodes for the model and the treatment train design section details how to connect source waters to the treatment train. Water flow rates (volumetric) and any constituent information required to calculate a unit process performance or cost must exist in the source water information.

The source water input dataset is arranged into the following columns:

- units: The units used for the constituent, such as kg/m3 (constituent concentration)
- value: The number of the variable of interest
- water\_type: The type/source of the water. This is where the intake unit water\_type names must match the train input water\_type process parameter in the treatment train design.
- case\_study: The treatment facility name.
- reference: The name of the project.
- variable: The name of the constituent or property of interest, such as 'flow' (required) or 'tds'.
- scenario: The name of the scenario that the values correspond with, otherwise the default value will be used.

## **Treatment Train Setup**

data/treatment\_train\_setup.csv

This is the input file used to arrange and connect unit processes in the proper order and with the proper flows to create a treatment train according to the user's design.

The columns are:

- CaseStudy: The treatment facility name.
- Reference: The name of the project that is using the model.
- **Scenario**: The name of the scenario that the values correspond with, used to match water recovery and constituent removal rates specific to the case study-scenario combination.
- **Unit**: The unit process to be added to the train. The unit name in this column must match the exact naming convention of the unit process in the WaterTAP3 model.
- **Type**: The role of the unit process along the treatment train.
  - Options are "intake", "treatment", "use", or "waste"
  - "intake" types are declared for units that begin the treatment train and require at least one source water.
  - "use" types are declared for units considered to have a treated water product. The volume of water that goes through these units is used to calculate LCOW. Therefore, there must be at least one unit declared as the use with a flow rate greater than zero. These units do not have an outlet or waste port connected to another unit (i.e. they are a terminal unit)
  - "treatment" types are declared for treatment units. These units can have any number of inlet, outlet, and waste ports.
  - "waste" types are declared for units that handle terminal waste streams for the facility. These units can have any number of inlet ports but don't have outlet or waste ports that connect to another unit (i.e. they are a terminal unit).
- UnitName: The unit process name as defined by the user.
  - Each unit name must be unique. For example, if there are two of the same unit processes under the **Unit** column (e.g. chlorination), the first chlorination unit name could be chlorination\_a and the second could be chlorination\_b. The unit in this column is connected to the unit defined in the **ToUnitName** column.
- **ToUnitName**: The **UnitName** for a unit process in a different row that connects to the **UnitName** for the current row. The user can include any number of destination units by including them in this column separated by a column and with *no space in between*.
  - Example: If the user wanted media\_filtration split outlet flow 50/50 to to and anti\_scalant\_addition chlorination\_b, they would put **ToUnitName** anit\_scalant\_addition,chlorination\_b in the column the media\_filtration row.
  - This is better explained in the example below.
- FromPort: For each unit process identified in the **ToUnitName** column, there needs to be a corresponding port, either "outlet" or "waste", that tells the model how to connect the current unit to the next unit in the train. If there is more than one port, the types are separated by a comma and *no space in between*.
  - Example: If the user wanted the treated flow from media\_filtration to go to anti\_scalant\_addition and the waste flow to go to backwash\_solids\_handling, put outlet, waste in the FromPort column for the media\_filtration row.

- Parameter: Used to characterize each unit process. All parameter formats are provided as python dictionaries, meaning the cell text must be enclosed by curly braces { }, have quotation marks around parameter names, commas between each parameter, and a colon : separating the parameter name and the value for that parameter.
  - Example: If "chemical\_name", and "dose" are the parameter names, the proper format is:
    - { 'chemical\_name': 'Chlorine', 'dose': 5}
  - Specifics for required and optional unit parameters for each unit are provided in the documentation for each unit model.
  - If the value for an input parameter is a word (e.g. chemical name), it *must* be in single ' ' or double " " quotes. If it is a number, it *must not* be in quotes.

## Treatment Train Example

Below is an example treatment train input file with various unit processes, flow splits, and waste streams.

1 CaseStudy	Reference	Scenario	Unit	Туре	UnitName	ToUnitName	FromPort	Parameter
<pre>2 example</pre>	nawi	baseline	well_field	intake	well_field	media_filtration	outlet	{'water_type': ['source_water']}
3 example	nawi	baseline	media_filtration	treatment	media_filtration	cartridge_filtration,anti_scalant_addition,landfill	outlet,outlet,waste	{'split_fraction': [0.65, 0.35]}
4 example	nawi	baseline	cartridge_filtration	treatment	cartridge_filtration	decarbonator	outlet	
5 example	nawi	baseline	anti_scalant_addition	treatment	anti_scalant_addition	ro_first_stage	outlet	{'dose': 5}
6 example	nawi	baseline	reverse_osmosis	treatment	ro_first_stage	decarbonator,ro_second_stage	outlet,waste	{'erd': 'no'}
7 example	nawi	baseline	reverse_osmosis	treatment	ro_second_stage	decarbonator,landfill	outlet,waste	{'erd': 'no'}
8 example	nawi	baseline	basic_unit	treatment	decarbonator	lime_softening	outlet	{'unit_process_name': 'decarbonator'}
9 example	nawi	baseline	lime_softening	treatment	lime_softening	chlorination	outlet	{'lime': 10}
10 example	nawi	baseline	chlorination	treatment	chlorination	treated_storage	outlet	{'chemical_name': 'Chlorine'}
11 example	nawi	baseline	holding_tank	treatment	treated_storage	municipal_drinking	outlet	{'avg_storage_time': 12, 'surge_cap': 0.2}
12 example	nawi	baseline	municipal_drinking	use	municipal_drinking			
13 example	nawi	baseline	landfill	waste	landfill			

- Row 2: well\_field is the "intake" unit for the treatment train. All the flow from the well\_field flows to media\_filtration.
  - "intake" units must have a water\_type in the **Parameter** column that corresponds to the proper source water found in case\_study\_water\_sources.csv
  - The source water name must be in quotes and enclosed in brackets [ ] even if there is only one source water for the treatment train. This is to facilitate the inclusion of multiple source waters for a single intake.
- Row 3: Outlets for media\_filtration flows to both cartridge\_filtration and ro\_first\_stage. There is also a waste stream that flows to landfill.
  - The user can designate any split fraction they want in the **Parameter** column by using the "split\_fraction" parameter.
  - Split fractions provided with "split\_fraction" must be provided in brackets [ ] and the order of values in the split fraction correspond to the order of units in **ToUnitName**. In this case, 65% of the flow from media\_filtration flows to cartridge\_filtration and 35% flows to anit scalant addition.
  - The unit paramater "split\_fraction" must be provided in **Parameter** even if the split is 50/50 (i.e. {'split\_fraction': [0.5, 0.5]}).
- Row 4: Flow from cartridge filtration flows to decarbonator.
  - Note that this flow stream is bypassing the two-stage reverse osmosis process. You can arrange flows in any configuration desired provided the input sheet is correct.

- Row 5: The chemical addition unit anti\_scalant\_addition receives 35% of flow from media\_filtration
  - This unit requires a "dose" in the Parameter column.
- Row 6: The permeate stream from ro\_first\_stage flows to decarbonator and the reject (i.e. waste) stream flows to ro\_second\_stage
  - Note that the **ToUnitName** column does not match the **Unit** column. The user can provide any name they want for the unit in **ToUnitName**, but the **Unit** entry must match *exactly* the name of the Python file for that unit (without '.py' appended)
  - In this case, because there are two reverse\_osmosis units, they must have different names for WaterTAP3 to correct the unit flows properly.
- Row 7: The permeate stream from ro\_second\_stage also flows to decarbonator and the reject (i.e. waste) stream flows to landfill
  - Both reverse\_osmosis units require an "erd" parameter to indicate if the model should include an energy recovery device.
- Row 8: The decarbonator is receiving flows from cartridge\_filtration, ro\_first\_stage, and ro\_second\_stage.
  - The decarbonator is a basic unit so must have a Parameter "unit\_process\_name" that matches the name of the desired unit in basic\_unit.csv.
  - More information on basic units is provided in the basic unit documentation.
- Row 9-11: For each of these rows, 100% of the flow from the UnitName is flowing to ToUnitName.
  - Each have entries in Parameters as required.
- Row 12: For this treatment train municipal\_drinking is the "use". Any water that flows through this unit is used to calculate LCOW.
  - The **ToUnitName** is empty for "use" units since flow does not go anywhere from here. It is a terminal unit. Similarly, it does not need an entry in **FromPort**

## **Water Recovery**

data/water\_revovery.csv

Water recovery *x* is represented as the fraction (between zero and one) of water recovered (treated) after it passes through a unit process. Case-study based water recovery is given for certain unit processes if the case study has a unique recovery rate, otherwise default values are used.

The water balance for a single unit incorporates the water recovery:

$$Q_{in}x = Q_{out}$$

And if the overall water balance for each unit is:

$$Q_{in} = Q_{out} + Q_{waste}$$

Then the water flow for the waste stream is:

$$Q_{waste} = Q_{in}(1-x)$$

The total system water recovery along a single stream in the train for all *n* units is the product of the water recovery for every unit in the stream:

$$x_{stream} = \prod_{i=1}^{n} x_i$$

And therefore the outlet flow for the entire stream the system water recovery multiplied by the sum of all k source flows to the system:

$$Q_{out,\,stream} = x_{stream} \sum_{i}^{k} Q_{in,\,i}$$

The columns of data/water\_recovery.csv are:

- case\_study: The treatment facility name or default
- scenario: The name of the scenario that the values correspond with
- unit\_process: The name of the unit process corresponding to the recovery value.
- recovery: How much water is recovered by each unit process (%)
- reference: The source of the recovery data

## **Constituent Removal**

data/constituent removal.csv

Constituent removal *r* is represented as the fraction (between zero and one) of the mass of the constituent being removed after it is passes through a unit process. Case-study based constituent removal is given for certain unit processes if the case study has a unique removal rate, otherwise default value are used.

The constituent removal data table states how much each unit process in each treatment facility removes a given water constituent. The model uses the information about the constituents in the source water as well as the removal rates of each unit process given in this constituent removal table to calculate constituent levels in the output water.

The overall mass balance for a single constituent *i* flowing into a single unit is based on volumetric flow and constituent concentration *c*:

$$Q_{in}c_{in,i} = Q_{out}c_{out,i} + Q_{waste}c_{waste,i}$$

Any mass removed by the unit is assumed to flow out the waste outlet. Then the constituent removal is:

$$Q_{in}c_{in,i}r_i = Q_{waste}c_{waste,i}$$

And therefore the mass flow out of the unit (i.e. to the next unit process) can be calculated with:

$$Q_{out}c_{out,i} = Q_{in}c_{in,i}(1-r_i)$$

The constituent removal input dataset is arranged into the following columns:

- case\_study: The treatment facility name.
- scenario: The name of the scenario associated with the removal fraction.
- units: The units used for the constituent, such as kg/m3 (constituent concentration).
- unit\_process: The unit process with the associated removal.
- value: The fraction or percent of the constituent in the source water that will be removed.
- constituent: The constituent being removed as named in the model.
- calculation\_type: How the model will handle the values when the unit process changes the constituent level, ultraviolet transmittance, or pH.
  - fractional\_constituent\_removal: fractional removal
  - absolute\_value: percent removal for ultraviolet transmittance
  - delta\_constituent\_or\_property: when the pH is changed
- reference: The name of the project that is using the mode
- data\_reference: The source of the data values and how values were calculated. Not used in the model but presented for user reference.
- constituent\_longform: The longform name of the constituent. Not used in the model but presented for user reference.

## **Financials**

This section describes the different costing and pipe parity metric outputs from WaterTAP3 and how they are calculated in the model.

## **Costing Indices and Factors**

Costing indices are available in plant\_cost\_indices.csv located in the data folder. The headings are:

- Year. The year for the costing index.
- Capital\_Index: The capital index for the given year.
- CatChem\_Index: The catalyst and chemical index for the given year.
- Labor\_Index: The labor index for the given year.
- CPI\_Index: The consumer price index (CPI) for the given year.

There are four types of cost indices applied in WaterTAP3 – Capital, Catalysts and Chemicals, Labor and Consumer Price Index. WaterTAP3 calculates each of these indices for 1990-2050. These factors are used to help account for the time-value of investments and are used in the capital and operating cost calculations. The following index factors are calculated for each process model in the treatment train based on:

- The user input for Analysis Year (for Cost Indices). This value is consistent across the entire treatment train.
- The Basis Year for the specific Process Model, Catalyst, Chemical, Replacement Part or other purchased item. This value is process-model-dependent with potentially different values across unit models within a treatment train.

The four cost indices are (where Y is the year):

Capital Cost Index Factor:

$$f_{cap} = \frac{Y_{analysis}}{Y_{model}}$$

Chemical Cost Index Factor:

$$f_{chem} = = \frac{Y_{analysis}}{Y_{chem}}$$

• Labor Cost Index Factor:

$$f_{labor} = \frac{Y_{analysis}}{Y_{model}}$$

• Other Cost Index Factor:

$$f_{other} = \frac{Y_{analysis}}{Y_{model}}$$

There are also various assumed costing factors for each case study read in from case\_study\_basis.csv:

Electricity price:

• Plant capacity utilization:

$$f_{util}$$

• Land cost as percent of FCI:

 $f_{land}$ 

• Working capital as percent of FCI:

 $f_{work}$ 

• Salaries as percent of FCI:

 $f_{sal}$ 

• Maintenance costs as percent of FCI:

 $f_{maint}$ 

• Laboratory costs as percent of FCI:

 $f_{lab}$ 

• Insurance/taxes as percent of FCI:

 $f_{ins}$ 

· Benefits as percent of salary:

 $f_{ben}$ 

• Assumed plant lifetime:

L

• Weighted Average Cost of Capital (debt interest rate):

WACC

## Financial Basis Inputs

The case study basis input data table contains the foundational technoeconomic assumptions for the entire treatment train.

The input dataset is arranged into the following columns:

- case\_study: The treatment facility name.
- scenario: The name of the scenario that the TEA values correspond with
- value: The number or name of the variable of interest
- reference: The name of the project that is using the model
- variable: The name of the variable of interest
  - analysis\_year. The first year of the plant is/was in operation
  - *location\_basis*: The country or U.S. state where the plant is located. Used for assigning the electricity cost [\$/kwh]. Electricity costs are provided in the data folder.

- plant\_life\_yrs: The initial design basis for plant-life and used for life cycle analysis calculations. The default plant-life is 20 years.
- land\_cost\_percent: The assumed cost of land as a percentage of total fixed capital investment. This is
  a part of the total capital investment.
- working\_capital\_percent: The assumed cost of working capital as a percentage of total fixed capital
  investment. This is a part of the total capital investment.
- salaries\_percent: The assumed cost of salaries as a percentage of total fixed capital investment. This
  is a part of the fixed operating costs.
- employee\_benefits\_percent: The assumed cost of employee benefits as a percentage of total salary cost. This is a part of the fixed operating costs.
- maintenance\_cost\_percent. The assumed cost of maintenance as a percentage of total fixed capital investment. This is a part of the fixed operating costs.
- laboratory\_fees\_percent: The assumed cost of laboratory fees as a percentage of total fixed capital investment. This is a part of the fixed operating costs.
- insurance\_and\_taxes\_percent: The assumed cost of insurance and taxes as a percentage of total fixed capital investment. This is a part of the fixed operating costs.
- default\_cap\_scaling\_exp: The typical value for economy-of-scale for capital equipment. This is a part of the total and fixed capital investment.
- default\_opex\_scaling\_exp: The typical value for economy-of-scale for fixed plant costs. This is a part
  of the fixed operating costs.
- cap\_by\_equity: The percent of the capital that is financed by equity rather than debt. This is a part of
  the capital recovery factor and LCOW calculations.
- debt\_interest\_rate: The rate for loan financing of capital. This is a part of the capital recovery factor and LCOW calculations.
- exp\_return\_on\_equity: The expected return, interest rate, or cost of capital associated with the portion of capital financed with equity.
- default\_tpec\_multiplier. The Total Purchased Equipment Cost (TPEC) to fixed capital investment. This is a part of the total and fixed capital investment calculations.
- default\_tic\_multiplier. The Total Installed Cost (TIC) to fixed capital investment. This is a part of the total and fixed capital investment calculations.

## System Capital Costs

The **Total Installed Costs (TIC)** are calculated for each individual unit process within the treatment train. This represents the cost of capital equipment plus the costs associated with installing the equipment in the plant. These include any costs associated with foundations, piping, insulation, assembly, buildings, electrical systems, and instrumentation. There are four approaches to calculating TIC in WaterTAP3, depending on the process, that vary in their level of detail:

- As a function of volumetric or mass flow only:
  - e.g. Basic units
- As function volumetric or mass flow and at least one other design criteria, such as chemical additions in which a
  dose is a required parameter:
  - · e.g. chemical additions
- Based on physical performance/attributes of unit model, such as water recovery or constituent removal:

- e.g. UV/AOP
- Multiple cost elements summed to calculate the TIC based on physical performance/attributes of unit model, such as pump and membrane costs for RO based on feed and osmotic pressures or evaporation pond costs that are based on evaporation rates, water recovery, and other design criteria:
  - e.g. Reverse osmosis

Depending on the costs assumed to be included in the unit's capital cost calculation (one of the four methods described above), some units may require additional cost multipliers to fully represent the TIC. For these units, the calculated capital cost is multiplied by either the **Equipment Installation Factor (EIF)** or the **Indirect Cost Factor (ICF)**. The EIF and ICF have default values of 3.4 (typical value range: 2.5-6.7) and 1.65 (typical value range: 1.2-1.7), respectively. After inclusion of either of these factors (if necessary), TIC is assumed to include indirect costs associated with constructing the process such as engineering costs, construction expenses, legal expenses, contractor fees, and contingencies. This is the **unadjusted Fixed Capital Investment**:

$$FCI_{unadi} = (EIF)TIC$$

Or:

$$FCI_{unadi} = (ICF)TIC$$

Then TIC is adjusted by the Capital Cost Index Factor (defined above) to get the FCI:

$$FCI = f_{cap}FCI_{unadi}$$

Finally, to arrive at the Total Capital Investment (TCI), land costs and the working capital are added to the FCI:

$$TCI = FCI + C_{land} + C_{work}$$

Where:

$$C_{land} = f_{land}FCI$$

And:

$$C_{work} = f_{work}FCI$$

## System Operating Costs

WaterTAP3 considers both variable and fixed operating costs. Variable operating costs are dependent on the flow rate and capacity utilization of each treatment technology, while fixed costs are dependent on the capital costs of the treatment facility.

#### Variable Operating Costs

Variable operating costs include any chemical additions, electricity costs, and other variable costs such as equipment replacements (e.g., membrane replacement costs for a reverse osmosis unit).

Chemical costs are based on the chemical dosage [kg/m3] as defined in the model or by the user for a given chemical addition. The costs of the chemicals can be found in the data folder. The annual chemical costs [\$MM/yr] are calculated as:

$$C_{chem} = \sum_{k}^{n} D_{k} C_{k} Q_{in} f_{util}$$

Where D is the dose [kg/m3] of chemical k and C is the unit cost [\$/kg] of chemical k as found in catalyst\_chemicals.csv.

Electricity costs are based on the electricity intensity [kWh/m3] of each unit process, which is provided as a constant or calculated based on the configuration of the treatment process (see unit models for details). The annual electricity costs [\$MM/yr] are calculated as:

$$C_{elec} = \sum_{k}^{n} E_{k} Q_{in} f_{util} P$$

Where E is the electricity intensity [kWh/m3] for unit k and P is the price of electricity for the locale [\$/kWh], taken from the electricity\_costs.csv data file.

There is also possibility for the inclusion of other operating costs that are unit specific. For most units, there are no costs included in this category.

## Fixed Operating Costs

Employee salaries are calculated and scaled according to:

$$C_{sal} = f_{labor} f_{sal} FCI_{unadi}$$

Employee benefits are calculated according to:

$$C_{ben} = C_{sal} f_{ben}$$

Plant maintenance costs are calculated as:

$$C_{maint} = f_{maint}FCI$$

Plant laboratory costs are calculated as:

$$C_{lab} = f_{lab}FCI$$

Plant insurance and taxes are calculated according to:

$$C_{ins} = f_{ins}FCI$$

### **Total & Annual Operating Costs**

The total fixed operating costs are calculated as:

$$C_{op, tot} = C_{sal} + C_{ben} + C_{maint} + C_{lab} + C_{ins}$$

And annual operating costs are:

$$C_{op, an} = C_{chem} + C_{elec} + C_{other} + C_{op, tot}$$

## **Pipe Parity Metrics**

## Levelized Cost of Water (LCOW)

The Levelized Cost Of Water (LCOW) [\$/m3] is one of the primary pipe-parity metrics provided as an output from WaterTAP3.

**Financials** 

$$LCOW = \frac{f_{recov}TCI + C_{op, an}}{Vf_{util}}$$

With the capital recovery factor:

$$f_{recov} = \frac{WACC(1 + WACC)^{L}}{(1 + WACC)^{L} - 1}$$

And V is the total volume of treated water that goes toward a beneficial use. In WaterTAP3, this is the volume of water that flows through any unit designated as a "use" in the input sheet treatment\_train\_setup.csv.

The individual components that sum to the total LCOW are calculated as:

$$LCOW_{TCI} = \frac{f_{recov}TCI}{V_{treat}f_{util}}$$

The electricity LCOW is calculated as:

$$LCOW_{elec} = \frac{C_{elec}}{V_{treat}f_{util}}$$

The fixed operating LCOW is calculated as:

$$LCOW_{op} = \frac{C_{op,an}}{V_{treat}f_{util}}$$

The chemical cost LCOW is calculated as:

$$LCOW_{chem} = \frac{C_{chem}}{V_{treat}f_{util}}$$

The other cost LCOW is calculated as:

$$LCOW_{other} = \frac{C_{other}}{V_{treat}f_{util}}$$

The electricity intensity for the system is calculated as:

$$E_{SYS} = \frac{C_{elec}}{PV_{treat}}$$

## **Unit Models**

All unit processes achieve the mass balances described in the Water Recovery and Constituent Removal section. The calculations of water recovery and constituent removal are based on factors (discussed in the Data Input for WaterTAP3 section) or equations that represent some level of the physical processes that occur in the treatment process. There are four levels of detail (discussed also in the Financials section) across the unit models.

## Agglomeration and Stacking

Agglomeration and stacking is the process of stacking metal-bearing ores for irrigation with a chemical solution.

#### **Unit Parameters**

There are two parameters:

- "mining\_capacity" mining capacity for the mine [tonnes/day]
  - Optional parameter
  - Default value is 922 tonnes/day
  - Must be provided with "ore\_heap\_soln" or default values for both will be used.
- "ore\_heap\_soln" volume of leach solution needed per mass ore [gal/tonne]
  - Optional parameter
  - Default value is 500 gal/tonne
  - Must be provided with "mining\_capacity" or default values for both will be used.

## **Capital Costs**

Capital costs for agglomeration and stacking and other associated mine units (i.e. Solution Distribution and Recovery Plant, Heap Leaching) are derived from Table 3 in Kappes (2002). The costing components explicitly calculated for these units via regressed data from this table are (associated WaterTAP3 unit in parentheses):

- Mining equipment (Heap Leaching)
- Mine development (Heap Leaching)
- Crushing plant (Heap Leaching)
- Leaching pads/ponds (Heap Leaching)
- · Agglomeration/stacking system (Agglomeration and Stacking)
- Solution distribution and recovery plant (Solution Distribution and Recovery Plant)

The costs from this table that are estimated as a fraction of the component costs are:

- Infrastructure (power, water, access roads, site office, service facilities)
- Owner's preproduction cost
- Engineering, procurement, construction management
- Import duties
- · Equipment and materials transport
- Initial operating supplies

Note that laboratory costs and working capital costs from this table are accounted for elsewhere in WaterTAP3 and so are excluded from the unit process calculations.

Capital costs for agglomeration and stacking are a function of the cost of the mining capacity X [tonnes/day]. This cost curve was derived from data for mining capacities of 3,000 tonnes/day and 15,000 tonnes/day from Table 3 in Kappes (2002):

$$C_{stack} = 0.00197X^{0.778}$$

To account for the other tabulated costing components in Table 3, WaterTAP3 calculates the fraction f that the other costs are of the component costs (i.e. other costs / component costs). The other costs fraction f are determined from a regression of the total cost in Table 3 minus the agglomeration and stacking costs (calculated above) vs. the mining capacities in that table (3,000 and 15,000 tonnes/day):

$$f = 0.3012X^{0.1119}$$

This fraction is multiplied by the agglomeration and stacking costs and added to those costs to form the costing basis:

$$C_{basis} = (C_{stack})(1+f)$$

To create a cost curve based on unit flow, WaterTAP3 scales the unit flow to 65 m3/hr (derived from the initial heap leaching case study used to develop WaterTAP3). The final cost curve for agglomeration and stacking is:

$$C_{agglom} = \frac{Q_{in}}{65} C_{basis}^{0.778}$$

## **Operating Costs**

The operating costs *P* [\$/year] for agglomeration and stacking are derived with cost curves regressed from data in Table 5 of Kappes (2002). Since this is the only component considered, this is the total operating cost:

$$P_{stack} = 6.28846X^{0.56932} = C_{op}$$

## **Electricity Intensity**

There is no electricity intensity associated with agglomeration and stacking.

#### References

Kappes, D.W. "Precious Metal Heap Leach Design and Practice" (2002)

in: Mineral processing plant design, practice, and control

pg. 1606-1630, ISBN: 0873352238

http://ore-max.com/pdfs/resources/precious\_metal\_heap\_leach\_design\_and\_practice.pdf

### Agglomeration and Stacking Module

class watertap3.wt\_units.agglom\_stacking.UnitProcess (\*args, \*\*kwds)

get\_costing (unit\_params=None, year=None)
Initialize the unit in WaterTAP3.

### **Alum Addition**

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

#### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

## **Capital Costs**

The chemical solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single alum addition unit, a = 15408 and b = 0.5479. The full cost equation in WaterTAP3 is:

$$C_{alum} = 15408S^{0.5479}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.15 in McGivney & Kawamura (2008).

## **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{alum} = Q_{in}D_{alum}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3] and ratio of the chemical in the solution [v/v]:

$$S = \frac{M_{alum}}{\rho_{alum} X_{alum}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as:

$$E_{alum} = \frac{0.746Sh}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

### **Assumptions**

• Number of units = 2

- Solution density [kg/m3] = 1360
- Ratio in solution = 0.5
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

### **Alum Addition Module**

```
class watertap3.wt_units.alum_addition.UnitProcess (*args, **kwds)
  elect()
    Electricity intensity.
        Parameters:
                           • lift_height (float) - Lift height for pump [ft]
                           • pump_eff (float) – Pump efficiency
                           • motor_eff (float) - Motor efficiency
            Returns:
                       Electricity intensity [kWh/m3]
  fixed_cap (unit_params)
    "unit_params" are the unit parameters passed to the model from the input sheet as a Python dictionary.
    EXAMPLE: {'dose': 10}
        Parameters:
                       dose (float) - Alum dose [mg/L]
                       Alum addition fixed capital cost [$MM]
            Returns:
  get_costing (unit_params=None, year=None)
    Initialize the unit in WaterTAP3.
  solution_vol_flow()
    Chemical solution flow in gal/day
        Parameters:
                           • solution_density (float) – Alum solution density [kg/m3]
                           • ratio_in_solution (float) - Ratio of alum in solution
            Returns: Alum solution flow [gal/day]
```

## Ammonia Addition

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

# **Capital Costs**

The ammonia solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a ammonia addition unit, a = 6699.1 and b = 0.4219. The full cost equation in WaterTAP3 is:

$$C_{amm} = 6699.15^{0.4219}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.11 in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{amm} = Q_{in}D_{amm}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3] and ratio of the chemical in the solution [v/v]:

$$S = \frac{M_{amm}}{\rho_{amm} X_{amm}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{amm} = \frac{0.746Sh}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

• Number of units = 2

- Solution density [kg/m3] = 1360
- Ratio in solution = 0.5
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

## Ammonia Addition Module

class watertap3.wt\_units.ammonia\_addition.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity.

Parameters:

- lift\_height (float) Lift height for pump [ft]
- pump\_eff (float) Pump efficiency
- motor\_eff (float) Motor efficiency

**Returns:** Electricity intensity [kWh/m3]

fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. EXAMPLE: {'dose': 10}

Fixed capital for ammonia addition is a function of ammonia dose, ammonia solution flow, and the number of units.

Parameters: dose (float) – Ammonia dose [mg/L]

**Returns:** Ammonia addition fixed capital cost [\$MM]

get\_costing (unit\_params=None, year=None)

Initialize the unit in WaterTAP3.

solution\_vol\_flow()

Chemical solution flow in gal/day

Parameters:

- solution\_density (float) Solution density [kg/m3]
- ratio\_in\_solution (float) Ratio of chemical in solution

Returns: Ammonia solution flow [gal/day]

# Anion Exchange

The anion exchange model in WaterTAP3 is based off of a regression of several runs using EPA's Work Breakdown Structure-Based (WBS EPA) model (see reference). These models incorporate several aspects of cost of the treatment process, including treatment, monitoring, and administrative costs. Both capital cost and electricity intensity are based entirely on volumetric flow, but are assumed to incorporate these costing aspects of the EPA model.

The WBS EPA models each have some "standard designs" that make default assumptions (see EPA documentation) and span a range of flows 0.03 MGD to 75 MGD. Influent sulfate (called tds\_in for WT3) also affects cost. The EPA model outputs several costing parameters, including total capital cost.

The approach for the WT3 model is to regress the total capital cost output from the EPA model vs. flow for each of vthe EPA model standard designs using influent TDS of 200, 600, and 1000 mg/L. The different capital costs for each of these model runs is determined from the TDS into the unit, which is determined dynamically by WaterTAP3 (e.g. the cost curve is different if the influent TDS is 100 mg/L vs. 900 mg/L). A similar approach is taken to determine electricity intensity.

Both sets of data are fit to a power curve:

$$Y = aQ^b$$

Where Q is the flows for the standard design EPA models. Then a and b are used with the flow in for the particular case study.

### **Unit Parameters**

None.

# **Capital Costs**

The cap\_total column is read in from the cost\_curves.csv based on influent TDS and is fit to the power curve described above. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$C_{ax} = aQ_{in}^b$$

## **Electricity Intensity**

The electricity\_intensity column is read in from the cost\_curves.csv based on influent TDS and is fit to the power curve described above. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$E_{ax} = aQ_{in}^b$$

#### Chemical Use

The WBS EPA model includes costs for sodium chloride and ion exchange resins. Rather than fit this data to a cost curve vs. standard design flows, the average is taken for the range of flows and assumed to be the "dose" for the particular chemical/material.

#### References

US Environmental Protection Agency (2017)

"Work Breakdown Structure-Based Cost Model for Anion Exchange Drinking Water Treatment" https://www.epa.gov/sites/production/files/2019-03/documents/wbs-anion-documentation-dec-2017\_v3.pdf

## Anion Exchange Module

class watertap3.wt\_units.anion\_exchange.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for anion exchange module [kWh/m3] :return:

# fixed\_cap (unit\_params)

Parameters:

- unit\_params (dict) Input parameters from input sheet.
- tds\_in (float) TDS into unit [mg/L]

Returns:

## **Anti-Scalant Addition**

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

# **Capital Costs**

The model assumes Hydrazine as the anti-scalant. This unit is based off of costing parameters for sulfuric acid.

The anti-scalant solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single anti-scalant addition unit, a = 900.97 and b = 0.6179. The full cost equation in WaterTAP3 is:

$$C_{anti} = 900.97S^{0.6179}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from FIGURE 5.5.11 - SULFURIC ACID FEED in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{anti} = Q_{in}D_{anti}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{anti}}{\rho_{anti}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{anti} = \frac{0.746Sh}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1021
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

## Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

## Anti-Scalant Addition Module

```
class watertap3.wt_units.anti_scalant_addition.UnitProcess (*args, **kwds)
  elect()
    Electricity intensity.
        Parameters:
                           • lift_height (float) - Lift height for pump [ft]
                           • pump_eff (float) – Pump efficiency
                           • motor_eff (float) - Motor efficiency
            Returns:
                       Electricity intensity [kWh/m3]
  fixed_cap (unit_params)
    "unit_params" are the unit parameters passed to the model from the input sheet as a Python dictionary.
    EXAMPLE: {'dose': 10}
            Returns: Anti-scalant addition fixed capital cost [$MM]
  get costing (unit params=None, year=None)
    Initialize the unit in WaterTAP3.
  solution_vol_flow()
    Chemical solution flow in gal/day
        Parameters: solution_density (float) – Solution density [kg/m3]
            Returns:
                       Anti-scalant solution flow [gal/day]
```

# **Backwash Solids Handling**

The backwash solids handling unit model represents the handling of the waste/backwash streams from filtration processes (e.g. tri-media filtration). It is typically recycled back into the treatment train or sent to a final waste unit.

## **Unit Parameters**

There is one parameter for backwash solids handling:

- "recovery" proportion of flow recycled back to treatment technology
  - Required parameter
  - Value between 0 and 1

# **Capital Costs**

The capital costs are a function of mass flow [kg/hr] from Figure 5.7.1 in in McGivney & Kawamura (2008):

$$C_{bw} = 9.76 \frac{M_{in}}{1577255}^{0.918}$$

The mass flow in is the sum of all the constituents flowing into the unit:

$$C_{in} = \sum_{i}^{n} c_{i}$$

Then, the density of the solution is [kg/m3]:

$$\rho_{in} = 0.6312(C_{in}) + 997.86$$

And mass flow is determined with [kg/hr]:

$$M_{in} = \rho_{in}Q_{in}$$

# **Electricity Intensity**

Electricity intensity for backwash solids handling is based off the pump used. The calculation includes:

• Lift height [ft]:

h

• The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

• And the influent flow in [gal/min] and [m3/hr]:

$$Q_{qpm}, Q_{m3hr}$$

Then the electricity intensity is calculated as:

$$E_{bw} = \frac{0.746Q_{gpm}h}{3960\eta_{pump}\eta_{motor}Q_{m3hr}}$$

# **Assumptions**

- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

## References

William McGivney & Susumu Kawamura (2008) Cost Estimating Manual for Water Treatment Facilities DOI:10.1002/9780470260036

# **Backwash Solids Handling Module**

class watertap3.wt\_units.backwash\_solids\_handling.UnitProcess (\*args, \*\*kwds)

# **Basic Unit**

Capital costs for the units defined as "basic" are based entirely on either the volumetric or mass flow into the unit. All of the data for each of the basic units is read in from the basic\_unit.csv located in the data folder.

### **Unit Parameters**

- "unit\_process\_name" unit process name that is being represented as a basic unit.
  - Required parameter
  - Must be enclosed in double " " or single ' ' quotes
  - Must match exactly the entry in the unit\_process column in basic\_unit.csv

### basic\_unit.csv

This .csv file contains all of the data used to calculate fixed capital costs and electricity intensity for all basic units. The columns are:

- unit\_process unit process name in WaterTAP3
- flow\_basis flow basis from costing source [m3/hr]
- cap\_basis B fixed capital investment from costing source [\$MM]
- cap\_exp x fixed capital investment scaling exponent
- elect electricity intensity for unit [kWh/m3]
- year costing basis year
- kind determines if unit is based on water flow or mass flow

# **Capital Costs**

#### Flow Based

Capital costs for basic units based on water flow are calculated with the general form:

$$C_{basic} = Bf^{x}$$

The ratio of the unit water flow to the basis water flow is the scaling factor *f* used to scale the unit costs to the basis costs:

$$f = \frac{Q_{in}}{Q_{basis}}$$

#### Mass Based

For those units based on mass flow, the mass flowing into the unit must be determined. First we determine the concentration flowing into the unit [kg/m3], calculated as the summation of the concentration of all constituents entering the unit:

$$C_{in} = \sum_{i}^{n} c_{i}$$

Then, we estimate the density of the solution [kg/m3] from Bartholomew & Mauter (2019):

$$\rho_{in} = 0.6312(C_{in}) + 997.86$$

Mass flow [kg/hr] is determined with:

$$M_{in} = \rho_{in}Q_{in}$$

Capital costs for basic units based on mass flow are calculated with the general form:

$$C_{basic} = Bf^{x}$$

The ratio of the unit mass flow to the basis mass flow is the scaling factor *f* used to scale the unit costs to the basis costs:

$$f = \frac{M_{in}}{M_{basis}}$$

# **Electricity Intensity**

Electricity intensity for basic units is read directly from the elect column in basic\_unit.csv (see above) and does not scale with flow (i.e. it is a fixed value).

## List of Basic Units

- Treatment Technologies:
  - ABMET Intermediate Pumps
  - ABMET Interstage Pumps
  - Aeration Basins
  - Air Floation
  - Anaerobic Digestion Oxidation
  - Bio-Active Filtration
  - Bioreactor
  - Bioreactor BW Pump
  - Bioreactor Feed Pump
  - Bioreactor Effluent Pump
  - Blending Reservoir
  - Buffer Tank
  - Conventional Activated Sludge (CAS)
  - Clarifier
  - Decarbonators
  - Dissolved Air Flotation (DAF)
  - Drainage Sump Pumps
  - Filter Presses
  - Intrusion Mitigation
  - Membrane Bioreactors (MBR)
  - Microscreen Filtration
  - Nanofiltration (NF)
  - pH Adjustment
  - Raw Water Pumps
  - Screens
  - Separators
  - Settling Ponds
  - Settling Tanks
  - SMP
  - Transfer Pumps
  - Tramp Oil Tanks
  - Ultrafiltration (UF)
  - Ultratiltration Feed Pumps
  - WAIV
  - Walnut Shell Filter
- Uses/Waste Streams & Other:

- Agriculture
- Cooling Supply
- Discharge
- Industrial
- Intrusion Mitigation
- Injection Wells
- Irrigation
- Mining
- Municipal WWTP
- Passthrough

#### References

Bartholomew, T. V. and M. S. Mauter (2019).

"Computational framework for modeling membrane processes without process and solution property simplifications." *Journal of Membrane Science* 573: 682-693.

## **Basic Unit Module**

```
class watertap3.wt_units.basic_unit.UnitProcess (*args, **kwds)
```

#### elect()

Electricity intensity for basic units.

**Returns:** Electricity intensity [kWh/m3]

fixed\_cap()

**Parameters:** flow\_in (float) – Flow in to basic unit [m3/hr]

# **Brine Concentrator**

The brine concentrator unit represents an evaporative (i.e. thermal) brine concentrator based on WateReuse Foundation (2008).

#### **Unit Parameters**

None.

## **Capital Costs**

Capital costs for brine concentrators are a function of influent TDS, water recovery, and flow in. The regression is based on data found in Tables 5.1 and A2.3 found in WateReuse Foundation (2008).

$$C_{brine} = 15.1 + 3.02 \times 10^{-4} (c_{TDS}) - 18.8(x_{wr}) + 8.08 \times 10^{-2} (Q_{in})$$

# **Electricity Intensity**

Electricity intensity is a function of the same variables and uses the same reference.

$$E_{brine} = 9.73 + 1.1 \times 10^{-4} (c_{TDS}) + 10.4 (x_{wr}) + 3.83 \times 10^{-5} (Q_{in})$$

### Reference

Mickley, Michael C. (2008)

"Survey of High-Recovery and Zero Liquid Discharge Technologies for Water Utilities"

WateReuse Foundation ISBN: 978-1-934183-08-3

#### **Brine Concentrator Module**

class watertap3.wt\_units.brine\_concentrator.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for brine concentrator.

#### Parameters:

- tds\_in (float) TDS concentration in to brine concentrator [mg/L]
- water\_recovery (float) Water recovery for the brince concentrator
- flow\_in (float) Water flow in to brine concentrator [m3/hr]

Returns: Electricity intensity [kWh/m3]

#### fixed\_cap()

Fixed capital for brine concentrator.

### Parameters:

- tds\_in (float) TDS concentration in to brine concentrator [mg/L]
- water\_recovery (float) Water recovery for the brine concentrator
- flow\_in (float) Water flow in to brine concentrator [m3/hr]

**Returns:** Fixed capital cost for brine concentrator [\$MM]

# **Cartridge Filtration**

#### **Unit Parameters**

None

# **Capital Costs**

The capital costs are a function of flow [MGD] with cost curve parameters from McGivney & Kawamura (2008):

$$C_{cart} = 0.72557Q_{in}^{0.5862}$$

# **Electricity Intensity**

Electricity intensity for cartridge filtration is fixed at 2E-4 kWh/m3 and is taken from Bukhary, et al. (2019).

#### References

#### **CAPITAL**

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

#### **ELECTRICITY**

Bukhary, S., Batista, J., Ahmad, S. (2019). An Analysis of Energy Consumption and the Use of Renewables for a Small Drinking Water Treatment Plant. *Water*, 12(1), 1-21.

## Cartridge Filtration Module

class watertap3.wt\_units.cartridge\_filtration.UnitProcess (\*args, \*\*kwds)

# Cation Exchange

The cation exchange model in WaterTAP3 is based off of a regression of several runs using EPA's Work Breakdown Structure-Based (WBS EPA) model (see reference). These models incorporate several aspects of cost of the treatment process, including treatment, monitoring, and administrative costs. Both capital cost and electricity intensity are based entirely on volumetric flow, but are assumed to incorporate these costing aspects of the EPA model.

The WBS EPA models each have some "standard designs" that make default assumptions (see EPA documentation) and span a range of flows 0.03 MGD to 75 MGD. Influent hardness (called tds\_in for WT3) also affects cost. The EPA model outputs several costing parameters, including total capital cost.

The approach for the WT3 model is to regress the total capital cost output from the EPA model vs. flow for each of vthe EPA model standard designs using influent TDS of 200, 600, and 1000 mg/L. The different capital costs for each of these model runs is determined from the TDS into the unit, which is determined dynamically by WaterTAP3 (e.g. the cost curve is different if the influent TDS is 100 mg/L vs. 900 mg/L). A similar approach is taken to determine electricity intensity.

Both sets of data are fit to a power curve:

$$Y = aQ^b$$

Where Q is the flows for the standard design EPA models. Then a and b are used with the flow in for the particular case study.

# **Unit Parameters**

None.

# **Capital Costs**

The cap\_total column is read in from the cost\_curves.csv based on influent TDS and is fit to the power curve described above. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$C_{cx} = aQ_{in}^b$$

## **Electricity Intensity**

The electricity\_intensity column is read in from the cost\_curves.csv based on influent TDS and is fit to the power curve described above. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$E_{cx} = aQ_{in}^{b}$$

#### Chemical Use

The WBS EPA model includes costs for sodium chloride and ion exchange resins. Rather than fit this data to a cost curve vs. standard design flows, the average is taken for the range of flows and assumed to be the "dose" for the particular chemical.

#### References

US Environmental Protection Agency (2017)

"Work Breakdown Structure-Based Cost Model for Cation Exchange Drinking Water Treatment" https://www.epa.gov/sites/production/files/2019-03/documents/wbs-cation-documentation-dec-2017\_v2.pdf

## Cation Exchange Module

class watertap3.wt\_units.cation\_exchange.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for cation exchange module [kWh/m3] :return:

# fixed\_cap()

Parameters:

- unit\_params (dict) Input parameters from input sheet.
- tds\_in (float) TDS into unit [mg/L]

Returns:

## Caustic Soda Addition

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

## Capital Costs:

The caustic soda flow S [galday] is used in a cost curve of the general form:

$$C = aS^b$$

For a single caustic soda addition unit, a = 2262.8 and b = 0.6195. The full cost equation in WaterTAP3 is:

$$C_{NaOH} = 2262.85^{0.6195}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.12b in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{NaOH} = Q_{in}D_{NaOH}$$

• The volumetric flow 'S' [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{NaOH}}{\rho_{NaOH} X_{NaOH}}$$

• The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{NaOH} = \frac{0.746Sh}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

## **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1021
- Ratio in solution = 50%
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

## Caustic Soda Addition Module

class watertap3.wt\_units.caustic\_soda\_addition.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity.

Parameters:

• lift\_height (float) – Lift height for pump [ft]

• pump\_eff (float) - Pump efficiency

• motor\_eff (float) - Motor efficiency

Returns: Electricity intensity [kWh/m3]

fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary.

EXAMPLE: {'dose': 10}

Parameters: dose (float) – Caustic dose [mg/L]

**Returns:** Caustic soda addition fixed capital cost [\$MM]

get\_costing (unit\_params=None, year=None)

Initialize the unit in WaterTAP3.

solution\_vol\_flow()

Chemical solution flow in gal/day

Parameters:

• solution\_density (float) - Solution density [kg/m3]

• ratio\_in\_solution (float) - Ratio of chemical in solution

Returns: Caustic soda solution flow [gal/day]

# Generic Chemical Addition

This unit is for a generic chemical addition that does not have a specific unit model in WaterTAP3.

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

You can add any chemical you want to catalyst\_chemicals.csv located in the data folder. The entry must include a price per kg and a year for the unit price.

#### **Unit Parameters**

There are four unit parameters:

- "chemical\_name" the name of the chemical to be added:
  - Required parameter
  - Must be in single ' ' or double " " quotes
  - Must match exactly an entry in catalyst\_chemicals.csv. If it is not in that file, users can easily add a chemical by providing an entry for each column.
- "dose" chemical dose [mg/L]:
  - Required parameter
  - · Dose of chemical to be added
- lift\_height" dynamic head for chemical pump [ft]:
  - Optional parameter
  - Default value is 100 ft
- "pump\_eff" and "motor\_eff" pump and motor efficiency:
  - Optional parameters
  - Default value for both is 0.9
  - Must be provided together or default value for both is used.

# **Capital Costs**

The generic chemical addition module is based off costing parameters for sulfuric acid.

The chemical solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single unit, a = 900.97 and b = 0.6179. The full cost equation in WaterTAP3 is:

$$C_{chem} = 900.975^{0.6179}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.11 in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{chem} = Q_{in}D_{chem}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{chem}}{\rho_{chem}}$$

• The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{chem} = \frac{0.7465h}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1000
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

## Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

#### **Chemical Addition Module**

class watertap3.wt\_units.chemical\_addition.UnitProcess (\*args, \*\*kwds)

elect (unit\_params)
Electricity intensity.

Parameters:

- **lift\_height** (*float*) Lift height for pump [ft]
- pump\_eff (float) Pump efficiency
- motor\_eff (float) Motor efficiency

**Returns:** Electricity intensity [kWh/m3]

fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. EXAMPLE: {'dose': 10}

Fixed capital for chemical addition is a function of chemical dose, chemical solution flow, and the number of units.

Parameters:

• chemical\_name (str) - Chemical name to be used.

• dose (float) - Dose of chemical [mg/L]

**Returns:** Chemical addition fixed capital cost [\$MM]

get\_costing (unit\_params=None, year=None)

Initialize the unit in WaterTAP3.

solution\_vol\_flow()

Chemical solution flow in gal/day

**Parameters:** solution\_density (float) – Solution density [kg/m3]

Returns: Chemical solution flow [gal/day]

# **Chlorination**

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

# **Unit Parameters**

There are two unit parameters:

- "chemical\_name" the name of the chemical for chlorination:
  - · Required parameter
  - Must be in single ' ' or double " " quotes
- "dose" chlorination dose [mg/L]:
  - Optional parameter
  - Default value is 9.5 mg/L (calculated below)

# **Capital Costs**

Chlorination capital costs are a function of the applied chlorine dose and the flow using data in Table 3.23 of the Texas Water Development Board (2016).

The chlorine dose is calculated from:

$$D_{CI} = C + rt + \frac{Ct}{t}$$

- C = Chlorine demand [mg/L]
- r = Chlorine decay rate [mg/Lhr]; default = 3
- t = Contact time [hr]; default = 1.5
- Ct = Desired Ct [mg\*min/L]; default = 450

Then, using the data provided in Table 3.23, cost data is read in based on the dose and fit to the general form based on flow [MGD]:

$$C = aQ^b$$

In other words, values of a and b will depend on the dose used for the unit. Once a and b are known, the capital costs for chlorination are:

$$C_{Cl} = aQ_{in}^b$$

## **Electricity Intensity**

Electricity intensity for chlorination is fixed at 5E-5 kWh/m3 and is taken from Bukhary, et al. (2019).

## **Assumptions**

According to the reference, capital costs only include chemical feed equipment and assume there is sufficient contact time downstream of the chlorine feed point.

## References

#### **CAPITAL**

#### User's Manual for Integrated Treatment Train Toolbox - Potable Reuse (IT3PR) Version 2.0

Steinle-Darling, E., Salveson, A., Russel, C., He, Q., Chiu, C., Lesan, D.

Texas Water Development Board

December 2016

## **ELECTRICITY**

Bukhary, S., Batista, J., Ahmad, S. (2019).

An Analysis of Energy Consumption and the Use of Renewables for a Small Drinking Water TreatmentPlant. *Water*, 12(1), 1-21.

## **Chlorination Module**

class watertap3.wt\_units.chlorination.UnitProcess (\*args, \*\*kwds)

# elect()

Electricity intensity.

**Returns:** Electricity intensity [kWh/m3]

fixed\_cap (unit\_params)

**Parameters:** unit\_params – Unit parameters from input sheet.

Returns:

# **Carbon Dioxide Addition**

## **Unit Parameters**

None

# **Capital Costs**

The capital costs are a function of flow [MGD] in McGivney & Kawamura (2008):

$$C_{co2} = 0.464Q_{in}^{0.7}$$

# **Electricity Intensity**

Electricity intensity is fixed at 0.01 kWh/m3 from \_\_\_\_\_

#### References

#### **CAPITAL**

William McGivney & Susumu Kawamura (2008) Cost Estimating Manual for Water Treatment Facilities DOI:10.1002/9780470260036

#### **ELECTRICITY**

# **Carbon Dioxide Addition Module**

class watertap3.wt\_units.co2\_addition.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity.

**Returns:** Electricity intensity [kWh/m3]

fixed\_cap()

# Coagulant Addition

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

# **Capital Costs**

The coagulant flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single alum addition unit, a = 15408 and b = 0.5479. The full cost equation in WaterTAP3 is:

$$C_{coag} = 15408S^{0.5479}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.15 in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{coag} = Q_{in}D_{coag}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{coag}}{\rho_{coag} X_{coag}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{coag} = \frac{0.746Sh}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1360

- Ratio in solution = 50%
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

# Coagulant Addition Module

Returns:

```
class watertap3.wt_units.coagulant_addition.UnitProcess (*args, **kwds)
  elect()
    Electricity intensity.
        Parameters:
                           • lift_height (float) - Lift height for pump [ft]
                           • pump_eff (float) - Pump efficiency
                           • motor_eff (float) - Motor efficiency
            Returns:
                       Electricity intensity [kWh/m3]
  fixed_cap (unit_params)
    "unit_params" are the unit parameters passed to the model from the input sheet as a Python dictionary.
    EXAMPLE: {'dose': 10}
    Fixed capital for alum addition is a function of alum dose, alum solution flow, and the number of units.
                      Alum addition fixed capital cost [$MM]
  get_costing (unit_params=None, year=None)
    Initialize the unit in WaterTAP3.
  solution_vol_flow()
    Chemical solution flow in gal/day
        Parameters:
                           • solution_density (float) - Solution density [kg/m3]
```

• ratio\_in\_solution (float) - Ratio of chemical in solution

Alum solution flow [gal/day]

# Crystallizer

The crystallizer represents a thermal crystallizer and is based on WateReuse Foundation (2008) data.

#### **Unit Parameters**

None.

## **Capital Costs**

Capital costs for crystallizers are a function of influent TDS, water recovery, and flow in.

The regression is based off of data found in Tables A2.1 and A2.3 found in WateReuse Foundation (2008).

$$C_{cryst} = 1.41 - 7.11 \times 10^{-7} (c_{TDS}) + 1.45 (x_{wr}) + 0.56 (Q_{in})$$

# **Electricity Intensity**

Electricity intensity is a function of the same variables and uses the same reference.

$$E_{crvst} = 56.7 + 1.83 \times 10^{-5} (c_{TDS}) - 9.47 (x_{wr}) - 8.63 \times 10^{-4} (Q_{in})$$

## Reference

Mickley, Michael C. (2008)

"Survey of High-Recovery and Zero Liquid Discharge Technologies for Water Utilities"

WateReuse Foundation ISBN: 978-1-934183-08-3

# Crystallizer Module

class watertap3.wt\_units.crystallizer.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for crystallizer.

Parameters:

- tds\_in (float) TDS concentration in to crystallizer [mg/L]
- water\_recovery (float) Water recovery for the crystallizer
- flow\_in (float) Water flow in to crystallizer [m3/hr]

**Returns:** Electricity intensity [kWh/m3]

#### fixed\_cap()

Fixed capital for crystallizer.

Parameters:

- tds\_in (float) TDS concentration in to crystallizer [mg/L]
- water\_recovery (float) Water recovery for the crystallizer
- flow\_in (float) Water flow in to crystallizer [m3/hr]

**Returns:** Fixed capital cost for crystallizer [\$MM]

# **Deep Well Injection**

Deep well injection is used to dispose of waste streams.

## **Unit Parameters**

Deep well injection has two parameters:

- "lift\_height" dynamic head for injection pump [ft]:
  - Optional parameter
  - Default value is 400 ft
- "pipe\_distance" pipe distance from facility to deep well injection site [mi]
  - · Required parameter

# **Capital Costs**

Capital costs for deep well injection are based off of the costs for the Kay Baily Hutchinson (KBH) deep well injection site. Costing calculation is split into well construction and pipe construction. From the KBH data, well construction is \$16.9 MM. Piping cost assumes an 8 in diameter pipe, and is calculated as:

$$C_{pipe} = 0.28x_{pipe}$$

The total fixed cost is then calculated by scaling with KBH flow according to:

$$C_{dwi} = (C_{well} + C_{pipe}) \frac{Q_{in}}{Q_{KBH}} 0.7$$

## **Electricity Intensity**

Electricity intensity for deep well injection is based off the pump used. The calculation includes:

• Lift height [ft]:

h

• The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

• And the influent flow in [gal/min] and [m3/hr]:

$$Q_{gpm}$$
,  $Q_{m3hr}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{dwi} = \frac{0.746Q_{gpm}h}{3960\eta_{pump}\eta_{motor}Q_{m3hr}}$$

# **Assumptions**

• Lift height [ft] = 100

- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

# Deep Well Injection Module

class watertap3.wt\_units.deep\_well\_injection.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for deep well injection [kWh/m3]

Parameters: lift\_height (float) - Lift height for pump [ft]

Returns: Electricity intensity [kWh/m3]

#### fixed\_cap (unit\_params)

Fixed capital cost for deep well injection.

#### Parameters:

- unit\_params (dict) Input parameter dictionary from input sheet.
- lift\_height (float) Lift height for pump [ft]
- pipe\_distance (float) Piping distance to deep well injection site

**Returns:** Fixed capital cost for deep well injection [\$MM]

# Electrodialysis Reversal

# **Unit Parameters**

None.

# **Capital Costs**

Capital costs for electrodialysis reversal are based on those from the Irwin case study.

$$C_{EDR} = 31 \frac{Q_{in}}{946}$$

# **Electricity Intensity**

Electricity intensity is a function of TDS [mg/L] into the unit and based off of a regression of data from Baker (2004):

$$E_{EDR} = 0.2534 + 5.149 \times 10^{-4} c_{tds}$$

## References

## **ELECTRICITY**

Richard W. Baker (2004)

"Membrane Technology and Applications, Second Edition"

DOI:10.1002/0470020393

# Electrodialysis Reversal Module

class watertap3.wt\_units.electrodialysis\_reversal.UnitProcess (\*args, \*\*kwds)

# **Evaporation Ponds**

Evaporation ponds are commonly used to further concentrate membrane brine to reduce the volume needed for disposal.

The generalized approach is as follows:

- 1. Calculate the evaporation rate based on environmental conditions.
- 2. Determine area required for evaporation ponds using a mass balance approach.
- Calculate capital costs based off of area and costing approach selected by user.

## **Unit Parameters**

The evaporation pond model draws from several sources and includes several optional parameters for user input. Further detail on these parameters is provided below:

- "approach" costing approach used for the model (more detail is provided below on each approach):
  - Optional parameter
  - Options are "wt3", "zld", and "lenntech"
  - Default approach is "wt3" if no input given
  - Must be enclosed in double " " or single ' ' quotes
- "evap\_method" method used to calculate evaporation rate
  - Optional parameter
  - Two options are "turc" and "jensen"
  - Defaults to "jensen" if no input given
  - Must be enclosed in double " " or single ' ' quotes
- "air\_temp" air temperature for evaporation rate calculation [C]
  - Optional parameter
  - Default value is 20 deg C
  - Note: Must provide both "air\_temp" and "solar\_rad" together or default values for both will be used.
- "solar\_rad" incident solar radiation for evaporation rate calculation [mJ/cm2]
  - Optional parameter
  - Default value is 25 mJ/cm2
  - Note: Must provide both "air\_temp" and "solar\_rad" together or default values for both will be used.
- "humidity" humidity for use in calculation of ratio to adjust pure water evaporation rate to saline water evaporation rate
  - Optional parameter
  - Default value is 0.5 (i.e. 50% humidity)

- Note: Must provide both "humidity" and "wind\_speed" together or default values for both will be used.
- "wind\_speed" wind speed for use in calculation of ratio to adjust pure water evaporation rate [m/s]
  - Optional parameter
  - Default value is 5 m/s
  - Note: Must provide both "humidity" and "wind\_speed" together or default values for both will be used.
- "liner\_thickness" thickness of liner used for calculation of cost per acre [mil]
  - Optional parameter
  - Default value is 50 mil
  - Note that 1 mil = 1/1000 inches
  - Note: Must provide "liner\_thickness", "land\_cost", "land\_clearing\_cost", and "dike\_height" together or default values for all will be used.
- "land\_cost" cost to purchase land for evaporation pond [\$/acre]
  - Optional parameter
  - Default value is \$5,000/acre
  - Note: Must provide "liner\_thickness", "land\_cost", "land\_clearing\_cost", and "dike\_height" together or default values for all will be used.
- "land\_clearing\_cost" cost to clear land for evaporation pond [\$/acre]
  - Optional parameter
  - Default value is \$1,000/acre
  - Note: Must provide "liner\_thickness", "land\_cost", "land\_clearing\_cost", and "dike\_height" together or default values for all will be used.
  - Typical costs for different types of land cover (Bureau of Reclamation, 2006):
    - brush = \$1,000/acre
    - sparsley wooded = \$2,000/acre
    - medium wooded = \$4,000/acre
    - heavily wooded = \$7,000/acre
- "dike\_height" height of dikes for evaporation pond [ft]
  - Default value is 8 ft
  - Typical dike heights are 4-12 ft (from Bureau of Reclamation reference)
  - Note: Must provide "liner\_thickness", "land\_cost", "land\_clearing\_cost", and "dike\_height" together or default values for all will be used.

## **Evaporation Rate Calculation**

The evaporation rate is *R* is dependent on site specific meteorological conditions and the salinity of the water. Salintiy has the effect of lowering the evaporation rate, and because evaporation ponds are commonliny used to concentrate brine streams, an evaporation rate calculated for pure water must be adjusted downward.

WaterTAP3 uses one of two regressions from each of the two references below to estimate the evaporation rate of pure water under the given meteorological conditions. Both are functions of air temperature T and solar irradiance J. For Jensen & Haise (1963) [mm/day]:

$$R_{pure} = R_{j\&h} = 0.41J(0.025T + 0.078)$$

And for Turc (1961) [mmday]:

$$R_{pure} = R_{turc} = \frac{0.313T(J+2.1)}{T+15}$$

In WaterTAP3, the water in the pond is assumed to be saline. The evaporation rate of saline water can be estimated to be 70% that of pure water (WateReuse Foundation, 2008). Thus, this calculated evaporation rate is multiplied by 0.7 to arrive at the estimated evaporation rate for saline water:

$$R_{saline} = 0.7R_{pure}$$

## **Pond Area Calculation**

For mass balance purposes in WaterTAP3, the flow of evaporated water is the considered to be the flow out of the unit. To accommodate a given water recovery, the area of the pond is calculated as:

$$A_{pond} = \frac{Q_{out}}{R_{saline}}$$

## **Capital Costs**

The user can choose one of three costing approaches for evaporation ponds in WaterTAP3 that can be provided as an option in unit\_params under "approach":

- 1. "wt3" default approach if the user does not provide one. Incorporates an adjusted pond area and more indepth costing function. Based on Bureau of Reclamation reference below.
- 2. "zld" only considers area and assumes \$0.3M/acre. Based on WateReuse reference below.
- 3. "lenntech" capital cost determined purely from flow. Based on Lenntech reference below.

#### WT3 Approach:

The WT3 approach is the default approach and uses a regression for total pond area from the Bureau of Reclamation reference below. After calculation of the required pond area based on flow above, if this approach is used the pond area is adjusted upwards to inorporate the additional area needed for dikes:

$$A_{adj} = 1.2(A_{pond})(1 + 0.155 \frac{h_{dike}}{\sqrt{A_{pond}}})$$

Then, the cost per acre [\$/acre] is determined that incorporates "liner\_thickness", "land\_cost", "land\_clearing\_cost", and "dike\_height":

$$C_{acre} = 5406 + 465(z_{liner}) + 1.07(z_{land}) + 0.931(z_{clear}) + 217.5(h_{dike})$$

Thus, using this approach capital costs for evaporation ponds are calculated as:

$$C_{evap} = A_{adi}C_{acre}$$

### ZLD Approach:

The ZLD approach is named from the WateReuse document it was adapted from. Using this approach, the unadjusted pond area is used. The cost per acre is assumed to be \$0.3MM. Thus, the capital costs are calculated as:

$$C_{evap} = A_{pond} \times 0.3$$

## Lenntech Approach:

This approach is based entirely on flow in [m3/d] to the evaporation pond and does not include the calculation for evaporation pond area. It assumes an evaporation rate of 1 m/yr:

$$C_{evap} = 0.031Q_{in}^{0.7613}$$

Note that while the reference mentions salt concentrations, land and earthwork costs, and liner costs, it is unclear how these are incorporated into the cost curve above.

# **Electricity Cost**

WaterTAP3 does not include any electricity intensity for evaporation ponds.

## References

#### **EVAPORATION RATE**

Turc, L. (1961)

"Water requirements assessment of irrigation, potential evapotranspiration:

Simplified and updated climatic formula."

Annales Agronomiques, 12, 13-49.

Jensen, M.E., Haise, H.R. (1963)

"Estimating evapotranspiration from solar radiation."

Proceedings of the American Society of Civil Engineers

Journal of the Irrigation and Drainage Division, vol. 89, pp. 15-41.

#### **COSTING**

U.S. Bureau of Reclamation (2006)

Mickley, Michael C.

"Membrane Concentrate Disposal: Practices and Regulation"

Chapter 10: Evaporation Pond Disposal

WateReuse Foundation (2008)

Mickley, Michael C.

"Survey of High-Recovery and Zero Liquid Discharge Technologies for Water Utilities"

ISBN: 978-1-934183-08-3

Lenntech.com

https://www.lenntech.com/Data-sheets/Brine-Evaporation-Ponds.pdf

## **Evaporation Pond Module**

class watertap3.wt units.evaporation pond.UnitProcess (\*args, \*\*kwds)

elect()

WaterTAP3 has no electricity intensity associated with evaporation ponds.

#### evaporation\_rate (unit\_params, t)

Calculation of evaporation rate [gpm/acre]

#### Parameters:

- unit\_params (dict) Input dictionary from input sheet.
- t (int) Time indexing variable to use in Var()
- evap\_method (str) Evaporation rate method
- humidity (float) Humidity expressed as decimal for evaporation rate calculation
- wind\_speed (float) Wind speed for evaporation rate calculation [m/s]
- air\_temp (float) Air temperature for evaporation rate calculation [C]
- solar\_rad (float) Incident solar radiation for evaporation rate calculation [mJ/m2]

#### Returns:

#### evaporation\_rate\_regress (t)

#### NOTE: THIS FUNCTION IS NOT USED IN THE CURRENT RELEASE OF WaterTAP3

Calculates evaporation rate based on air temperature, TDS in, humidity, and wind speed.

#### fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. Evaporation ponds can have many unit\_params

EXAMPLE: {'approach': 'wt3', 'area': 3500, 'humidity': 0.75, 'wind\_speed': 10}

#### Parameters:

- unit\_params (dict) Input parameter dictionary from input sheet.
- liner\_thickness (float) Liner thickness [mil]
- land\_cost (float) Cost of land for evaporation pond [\$/acre]
- land\_clearing\_cost (float) Cost to clear land for evaporation pond [\$/acre]
- dike\_height (float) Height of dikes [ft]

**Returns:** Fixed capital cost for evaporation ponds [\$MM]

## Ferric Chloride Addition

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

## **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

# **Capital Costs**

The ferric chloride solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single ferric chloride addition unit, a = 34153 and b = 0.319. The full cost equation in WaterTAP3 is:

$$C_{ferric} = 34153S^{0.319}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.13 in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{ferric} = Q_{in}D_{ferric}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{ferric}}{\rho_{ferric} X_{ferric}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{ferric} = \frac{0.746Sh}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1460

- Ratio in solution = 42%
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

#### Ferric Chloride Addition Module

```
class watertap3.wt_units.ferric_chloride_addition.UnitProcess (*args, **kwds)
  elect()
    Electricity intensity.
         Parameters:
                           • lift_height (float) - Lift height for pump [ft]
                           • pump_eff (float) - Pump efficiency
                           • motor_eff (float) - Motor efficiency
            Returns:
                       Electricity intensity [kWh/m3]
  fixed_cap (unit_params)
    "unit_params" are the unit parameters passed to the model from the input sheet as a Python dictionary.
    EXAMPLE: {'dose': 10}
    Fixed capital for ferric chloride addition is a function of ferric dose, ferric solution flow, and the number of units.
                      Ferric addition fixed capital cost [$MM]
  get_costing (unit_params=None, year=None)
    Initialize the unit in WaterTAP3.
  solution_vol_flow()
    Chemical solution flow in gal/day
         Parameters:
                           • solution_density (float) - Solution density [kg/m3]
                           • ratio_in_solution (float) - Ratio of chemical in solution
            Returns:
                      Ferric solution flow [gal/day]
```

# Fixed Bed Gravity Basin

The fixed bed gravity basin unit in WaterTAP3 is based off of a regression of several runs using EPA's Work Breakdown Structure-Based (WBS EPA) model. These models each have some "standard designs" that make default assumptions and span a range of flows 0.03 MGD to 75 MGD (USEPA (2019)).

The approach for the WT3 model is to regress the total capital cost output from the EPA model vs. flow for each of the EPA model standard designs with the fixed bed gravity basin option. A similar approach is taken to determine electricity intensity.

Both sets of data are fit to a power curve. Then a and b are used with the flow for the model to determine capital and electricity intensity.

#### **Unit Parameters**

None.

# **Capital Costs**

The cap\_total column is read in from the cost\_curves.csv and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$C_{fbgb} = aQ_{in}^{b}$$

# Electricity Intensity

The electricity\_intensity column is read in from the cost\_curves.csv and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine electricity intensity:

$$E_{fbgb} = aQ_{in}^b$$

#### Chemical Use

The WBS EPA model includes costs for acetic acid, phosphoric acid, iron chloride, activated carbon, sand, and anthracite. The average is taken for the range of flows and assumed to be the "dose" for the particular chemical/material.

#### References

US Environmental Protection Agency (2019)

"Work Breakdown Structure-Based Cost Model for Biological Drinking Water Treatment" https://www.epa.gov/sites/production/files/2019-07/documents/wbs-biotreat-documentation-june-2019.pdf https://www.epa.gov/sdwa/drinking-water-treatment-technology-unit-cost-models

### Fixed Bed Gravity Basin Module

class watertap3.wt\_units.fixed\_bed\_gravity\_basin.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for fixed bed gravity basin [kWh/m3] :return:

fixed\_cap()

**Returns:** Fixed capital for fixed bed gravity basin [\$MM]

### Fixed Bed Pressure Vessel

The fixed bed gravity basin unit in WaterTAP3 is based off of a regression of several runs using EPA's Work Breakdown Structure-Based (WBS EPA) model. These models each have some "standard designs" that make default assumptions and span a range of flows 0.03 MGD to 75 MGD (USEPA (2019)).

The approach for the WT3 model is to regress the total capital cost output from the EPA model vs. flow for each of the EPA model standard designs with the fixed bed pressure vessel option. A similar approach is taken to determine electricity intensity.

Both sets of data are fit to a power curve. Then a and b are used with the flow for the model to determine capital and electricity intensity.

#### **Unit Parameters**

None

# **Capital Costs**

The cap\_total column is read in from the cost\_curves.csv and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$C_{fbpv} = aQ_{in}^b$$

# **Electricity Intensity**

The electricity\_intensity column is read in from the cost\_curves.csv and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine electricity intensity:

$$E_{fbpv} = aQ_{in}^b$$

#### Chemical Use

The WBS EPA model includes costs for acetic acid, phosphoric acid, iron chloride, activated carbon, sand, and anthracite. The average is taken for the range of flows and assumed to be the "dose" for the particular chemical/material.

#### References

US Environmental Protection Agency (2019)

"Work Breakdown Structure-Based Cost Model for Biological Drinking Water Treatment" https://www.epa.gov/sites/production/files/2019-07/documents/wbs-biotreat-documentation-june-2019.pdf https://www.epa.gov/sdwa/drinking-water-treatment-technology-unit-cost-models

### Fixed Bed Pressure Vessel Module

class watertap3.wt\_units.fixed\_bed\_pressure\_vessel.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for fixed bed pressure vessel [kWh/m3] :return:

fixed\_cap()

Returns: Fixed capital for fixed bed pressure vessel [\$MM]

# **GAC** - Gravity

The gravity GAC unit in WaterTAP3 is based off of a regression of several runs using EPA's Work Breakdown Structure-Based (WBS EPA) model. These models each have some "standard designs" that make default assumptions and span a range of flows 0.03 MGD to 75 MGD (USEPA (2019)).

The approach for the WT3 model is to regress the total capital cost output from the EPA model vs. flow for each of the EPA model standard designs with the gravity GAC option. A similar approach is taken to determine electricity intensity.

Both sets of data are fit to a power curve. Then a and b are used with the flow for the model to determine capital and electricity intensity.

#### **Unit Parameters**

Anion exchange has one parameter:

- "ebct" empty bed contact time for the unit [min]:
  - Required parameter
  - There are different costing data for 0-60 min and >60 min

### **Capital Costs**

The cap\_total column is read in from the cost\_curves.csv based on user-defined EBCT and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$C_{qac} = aQ_{in}^b$$

# **Electricity Intensity**

The electricity\_intensity column is read in from the cost\_curves.csv based on user-defined EBCT and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine electricity intensity:

$$E_{aac} = aQ_{in}^b$$

#### Chemical Use

The WBS EPA model includes costs for activated carbon. The average is taken for the range of flows and assumed to be the "dose" for the particular chemical/material.

#### References

US Environmental Protection Agency (2017)

"Work Breakdown Structure-Based Cost Model for Granular Activated Carbon Drinking Water Treatment" https://www.epa.gov/sites/production/files/2019-03/documents/wbs-gac-documentation-dec-2017\_v2.pdf https://www.epa.gov/sdwa/drinking-water-treatment-technology-unit-cost-models

## **GAC - Gravity Module**

class watertap3.wt\_units.gac\_gravity.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity gravity GAC [kWh/m3] :return:

fixed\_cap (unit\_params)

Returns: Fixed capital for gravity GAC [\$MM]

## GAC - Pressure Vessel

The GAC pressure vessel in WaterTAP3 is based off of a regression of several runs using EPA's Work Breakdown Structure-Based (WBS EPA) model. The WBS EPA models each have some "standard designs" that make default assumptions (USEPA (2019)) and span a range of flows 0.03 MGD to 75 MGD.

The approach for the WT3 model is to regress the total capital cost output from the EPA model vs. flow for each of the EPA model standard designs with the fixed bed gravity basin option. A similar approach is taken to determine electricity intensity.

Both sets of data are fit to a power curve. Then a and b are used with the flow for the model.

#### **Unit Parameters**

Anion exchange has one parameter:

- "ebct" empty bed contact time for the unit [min]:
  - Required parameter
  - There are different costing data for 0-60 min and >60 min

## **Capital Costs**

The cap\_total column is read in from the cost\_curves.csv based on user-defined EBCT and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine capital costs:

$$C_{gac} = aQ_{in}^b$$

# **Electricity Intensity**

The electricity\_intensity column is read in from the cost\_curves.csv based on user-defined EBCT and is fit to a power curve. Then a and b from that regression is used with the unit flow [m3/hr] to determine electricity intensity:

$$E_{aac} = aQ_{in}^b$$

### Chemical Use

The WBS EPA model includes costs for activated carbon. The average is taken for the range of flows and assumed to be the "dose" for the particular chemical/material.

#### References

US Environmental Protection Agency (2017)

"Work Breakdown Structure-Based Cost Model for Granular Activated Carbon Drinking Water Treatment" https://www.epa.gov/sites/production/files/2019-03/documents/wbs-gac-documentation-dec-2017\_v2.pdf https://www.epa.gov/sdwa/drinking-water-treatment-technology-unit-cost-models

## GAC - Pressure Vessel Module

```
class watertap3.wt_units.gac_pressure_vessel.UnitProcess (*args, **kwds)
```

elect()

Electricity intensity for pressure vessel GAC [kWh/m3] :return:

```
fixed_cap (unit_params)
```

**Returns:** Fixed capital for pressure vessel GAC [\$MM]

# Heap Leaching

Heap leaching is the process of collecting the leached solution irrigated over a stack of metal-bearing ores.

#### **Unit Parameters**

There are two parameters:

- "mining\_capacity" mining capacity for the mine [tonnes/day]
  - Optional parameter
  - Default value is 922 tonnes/day
  - Must be provided with "ore\_heap\_soln" or default values for both will be used.
- "ore\_heap\_soln" volume of leach solution needed per mass ore [gal/tonne]
  - Optional parameter
  - Default value is 500 gal/tonne
  - Must be provided with "mining\_capacity" or default values for both will be used.

### **Capital Costs**

Capital costs for heap leaching and other associated mine units (i.e. Solution Distribution and Recovery Plant, Agglomeration and Stacking) are derived from Table 3 in Kappes (2002). The costing components explicitly calculated for these units via regressed data from this table are (associated WaterTAP3 unit in parentheses):

- Mining equipment (Heap Leaching)
- Mine development (Heap Leaching)
- · Crushing plant (Heap Leaching)
- Leaching pads/ponds (Heap Leaching)
- Agglomeration/stacking system (Agglomeration and Stacking)
- Solution distribution and recovery plant (Solution Distribution and Recovery Plant)

The costs from this table that are estimated via different method below are:

- Infrastructure (power, water, access roads, site office, service facilities)
- Owner's preproduction cost
- Engineering, procurement, construction management
- Import duties
- · Equipment and materials transport
- · Initial operating supplies

Note that laboratory costs and working capital costs from this table are accounted for elsewhere in WaterTAP3 and so are excluded from the unit process calculations.

Capital costs for heap leaching are a function of the mining equipment, mine development, the crushing plant, and the leaching pads/ponds. Each of these are a function of the mining capacity *X* [tonnes/day]. Cost curves for these components were derived from data for mining capacities of 3,000 tonnes/day and 15,000 tonnes/day from Table 3 in Kappes (2002):

$$C_{equip} = 0.00124X^{0.93454}$$

$$C_{devel} = 0.01908X^{0.43068}$$

$$C_{crush} = 0.0058X^{0.6651}$$

$$C_{leach} = 0.0005X^{0.94819}$$

To account for the other tabulated costing components in Table 3, WaterTAP3 calculates the fraction f that the other costs are of the component costs (i.e. other costs / component costs). The other costs fraction f are determined from a regression of the total cost in Table 3 minus the sum of the heap leaching costs (calculated above) vs. the mining capacities in that table (3,000 and 15,000 tonnes/day):

$$f = 0.3012X^{0.1119}$$

This fraction is multiplied by the sum of the component costs (calculated above) and added to that sum. This is the costing basis for Heap Leaching:

$$C_{basis} = (C_{equip} + C_{devel} + C_{crush} + C_{leach})(1 + f)$$

To create a cost curve based on unit flow, WaterTAP3 scales the unit flow to 73 m3/hr (derived from the initial heap leaching case study used to develop WaterTAP3) and creates an exponent *b* from:

$$b = \frac{0.935C_{equip} + 0.431C_{devel} + 0.665C_{crush} + 0.948C_{leach}}{C_{equip} + C_{devel} + C_{crush} + C_{leach}}$$

Note that the coefficients in the numerator of the above equation are the exponents for the cost curves for each costing component.

And then the final capital costing curve for heap leaching unit is:

$$C_{heap} = \frac{Q_{in}}{73} C_{basis}^b$$

## **Operating Costs**

The operating costs P [\$/year] for heap leaching are derived with cost curves regressed from data in Table 5 of Kappes (2002). Included for heap leaching in WaterTAP3 are operational costs relating to:

- Mining equipment
- Crushing plant
- Leaching pads/ponds

These cost curves are:

$$P_{mining} = 22.54816X^{0.74807}$$
  
 $P_{crush} = 4.466X^{0.8794}$   
 $P_{leach} = 6.34727X^{0.68261}$ 

The total operating cost is the sum of these components:

$$C_{op} = P_{mining} + P_{crush} + P_{leach}$$

### **Electricity Intensity**

There is no electricity intensity associated with heap leaching.

#### References

Kappes, D.W. "Precious Metal Heap Leach Design and Practice" (2002)

in: Mineral processing plant design, practice, and control

pg. 1606-1630, ISBN: 0873352238

 $http://ore-max.com/pdfs/resources/precious\_metal\_heap\_leach\_design\_and\_practice.pdf$ 

# Heap Leaching Module

class watertap3.wt\_units.heap\_leaching.UnitProcess (\*args, \*\*kwds)

# **Hydrochloric Acid Addition**

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

# **Capital Costs**

The hydrochloric acid solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single hydrochloric acid addition unit, a = 900.97 and b = 0.6179. The full cost equation in WaterTAP3 is:

$$C_{HCI} = 900.975^{0.6179}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.11 in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{HCI} = Q_{in}D_{HCI}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{HCI}}{\rho_{HCI}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{HCI} = \frac{0.7465h}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1490

- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

# Hydrochloric Acid Addition Module

```
class watertap3.wt_units.hydrochloric_acid_addition.UnitProcess (*args, **kwds)
  elect()
    Electricity intensity.
        Parameters:
                           • lift_height (float) - Lift height for pump [ft]
                           • pump_eff (float) – Pump efficiency
                           • motor_eff (float) - Motor efficiency
            Returns:
                       Electricity intensity [kWh/m3]
  fixed_cap (unit_params)
    "unit_params" are the unit parameters passed to the model from the input sheet as a Python dictionary.
    EXAMPLE: {'dose': 10}
            Returns: HCl addition fixed capital cost [$MM]
  get_costing (unit_params=None, year=None)
    Initialize the unit in WaterTAP3.
  solution_vol_flow()
    Chemical solution flow in gal/day
        Parameters:
                       solution_density (float) – Solution density [kg/m3]
            Returns:
                       HCl solution flow [gal/day]
```

# Iron & Manganese Removal

The Fe/Mn removal unit in WaterTAP3 is based off of the dual media filtration schematic in the Lenntech reference using costing data in McGivney & Kawamura (2008).

### **Unit Parameters**

None

# **Capital Costs**

The coagulation/flocculation unit in WaterTAP3 includes costing for filtration media, backwash system, and air blower.

$$C_{Fe/Mn} = (C_{filt} + C_{bw} + nC_{blow}) \frac{Q_{in}}{4732} ^{0.7}$$

Filtration capital is a function of media surface area and calculated with:

$$C_{filt} = 21377 + 38.319A$$

Backwash capital is also a function of media surface area:

$$C_{bw} = 92947 + 292.44A$$

The blower capital is assumed.

# **Assumptions**

There are six units:

$$n = 6$$

The filter surface area is 6243 ft2:

$$A = 6243$$

The air/water ratio in the blower is 0.001 [v/v]:

$$r = 0.001$$

The capital for the air blower is \$100,000:

$$C_{blow} = 100000$$

# Electricity Intensity

The total electricity intensity for Fe/Mn removal is from the blower [kWh/m3]:

$$E_{Fe/Mn} = \frac{p_{blow}}{Q_{in}}$$

Where blower power is calculated with [hp]:

$$p_{rm} = 147.8q_{air}$$

And the air flow rate is [m3/hr]:

$$q_{air} = Q_{in}r$$

### References

William McGivney & Susumu Kawamura (2008) Cost Estimating Manual for Water Treatment Facilities DOI:10.1002/9780470260036

Schema of an iron removal system

https://www.lenntech.com/schema-of-an-iron-removal-system.htm

# Iron & Manganese Removal Module

class watertap3.wt\_units.iron\_and\_manganese\_removal.UnitProcess (\*args, \*\*kwds)

## Landfill

#### **Unit Basics**

This unit is a terminal unit in WaterTAP3 and represents the cost of sending residual solids to landfill.

#### **Unit Parameters**

None.

# **Capital Costs**

Landfill costs are a function of mass flow into the unit:

$$C_{lf} = \frac{M_{in}}{100000} 0.7$$

The mass flow is calculated by first calculating the total concentration flowing into the unit:

$$C_{in} = \sum_{i}^{n} c_{i}$$

Then, we estimate the density of the solution [kg/m3]:

$$\rho_{in} = 0.6312(C_{in}) + 997.86$$

Mass flow [kg/hr] is determined with:

$$M_{in} = \rho_{in}Q_{in}$$

## **Electricity Intensity**

There are no electricity costs associated with landfill in WaterTAP3.

### References

#### Landfill Module

class watertap3.wt\_units.landfill.UnitProcess (\*args, \*\*kwds)

### Landfill ZLD

#### **Unit Basics**

This unit is a terminal unit in WaterTAP3 and represents the cost of sending residual solids to landfill.

#### **Unit Parameters**

None.

# **Capital Costs**

Landfill ZLD costs are a function of mass flow into the unit:

$$C_{lf} = \frac{M_{in}}{302096} 0.7$$

The mass flow is calculated by first calculating the total concentration flowing into the unit:

$$C_{in} = \sum_{i}^{n} c_{i}$$

Then, we estimate the density of the solution [kg/m3]:

$$\rho_{in} = 0.6312(C_{in}) + 997.86$$

Mass flow [kg/hr] is determined with:

$$M_{in} = \rho_{in}Q_{in}$$

## **Electricity Intensity**

There are no electricity costs associated with landfill ZLD in WaterTAP3.

### References

Mickley, Michael C. (2008)

"Survey of High-Recovery and Zero Liquid Discharge Technologies for Water Utilities"

WateReuse Foundation ISBN: 978-1-934183-08-3

### Landfill ZLD Module

class watertap3.wt\_units.landfill\_zld.UnitProcess (\*args, \*\*kwds)

### **Lime Addition**

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

- "lime" dose of lime [mg/L]
  - Required parameter

# **Capital Costs**

The lime solution mass flow M [lb/day] is used in a cost curve of the general form:

$$C = aM^b$$

For a single lime addition unit, a = 16972 and b = 0.5435. The full cost equation in WaterTAP3 is:

$$C_{lime} = 16972S^{0.5435}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.9 in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/hr] of the solution necessary to achieve the desired dose:

$$M_{lime} = Q_{in}D_{lime}$$

• The volumetric flow S [m3/hr] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{lime}}{\rho_{lime}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{lime} = \frac{0.746Sh}{3960 \eta_{pump} \eta_{motor} Q_{in}}$$

# **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1250
- Lift height [ft] = 100

- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### Reference

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

### Lime Addition Module

```
class watertap3.wt_units.lime_addition.UnitProcess (*args, **kwds)
elect ()
    Electricity intensity.
    Parameters:
    • lift_height (float) - Lift height for pump [ft]
```

• pump\_eff (float) – Pump efficiency

• motor\_eff (float) - Motor efficiency

Returns: Electricity intensity [kWh/m3]

fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. EXAMPLE: {'lime': 10}

Fixed capital for lime addition is a function of lime dose, lime solution flow, and the number of units.

**Parameters: lime** (*float*) – Lime dose [mg/L]

**Returns:** Lime addition fixed capital cost [\$MM]

get\_costing (unit\_params=None, year=None)
Initialize the unit in WaterTAP3.

solution\_vol\_flow()

Chemical solution flow in gal/day

**Parameters:** solution\_density (float) – Solution density [kg/m3]

Returns: Lime solution vol. flow [gal/day], Lime solution mass flow [lb/day]

# **Lime Softening**

### **Unit Parameters**

There is one unit parameter:

- "lime" lime dose for unit [mg/L]:
  - Required parameter

# **Capital Costs**

The capital costs are a function of flow [m3/hr] with cost curve parameters from the Minnesota Rural Water Association.

$$C_{lime} = 0.0704Q_{in}^{0.7306}$$

# **Electricity Intensity**

Electricity intensity for lime softening is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/hr] of the solution necessary to achieve the desired dose:

$$M_{lime} = Q_{in}D_{lime}$$

• The volumetric flow S [m3/hr] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{lime}}{\rho_{lime}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{lime} = \frac{0.7465h}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

- Solution density [kg/m3] = 1250
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### References

Minnesota Rural Water Association, Chapter 16 Lime Softening https://www.mrwa.com/WaterWorksMnl/Chapter%2016%20Lime%20Softening.pdf

# Lime Softening Module

class watertap3.wt\_units.lime\_softening.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for chemical additions is a function of lift height, pump efficiency, and motor efficiency.

**Returns:** Electricity intensity [kWh/m3]

fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. EXAMPLE: {'lime': 10}

Fixed capital for lime addition is a function of lime dose, lime solution flow, and the number of units.

**Parameters: lime** (*float*) – Lime dose [mg/L]

Returns: Lime addition fixed capital cost [\$MM]

get\_costing (unit\_params=None, year=None)

Initialize the unit in WaterTAP3.

solution\_vol\_flow()

Determine alum solution flow rate in gal / day

Returns: Lime solution flow [gal/day]

### Media Filtration

#### **Unit Parameters**

None

## **Capital Costs**

Capital costs for media filtration includes the cost of the filter and the cost of the backwash system (McGivney & Kawamura (2008)).

$$C_{mf} = C_{filter} + C_{bw}$$

The cost of the filter is a function of the surface area and the number of units:

$$C_{filter} = (21377 + 38.319A)n$$

With the filter surface area calculated with the assumed filtration rate [ft2]:

$$A = \frac{Q_{in}}{V}$$

The cost of the backwash system is also a function of filter surface area:

$$C_{bw} = 92947 + 292.44A$$

### **Assumptions**

There are six units:

$$n = 6$$

The filtration rate is 10 m/hr:

$$v = 10$$

## **Electricity Intensity**

Electricity intensity is fixed at 0.00015 kWh/m3 from Bukhary et al. (2019).

### References

### **CAPITAL**

William McGivney & Susumu Kawamura (2008)
Cost Estimating Manual for Water Treatment Facilities
DOI:10.1002/9780470260036

#### **ELECTRICITY**

Bukhary, S., et al. (2019).

"An Analysis of Energy Consumption and the Use of Renewables for a Small Drinking Water Treatment Plant." Water 12(1).

### Media Filtration Module

class watertap3.wt\_units.media\_filtration.UnitProcess (\*args, \*\*kwds)

## Microfiltration

#### **Unit Parameters**

None

## **Capital Costs**

Capital costs for microfiltration is based entirely on flow [MGD] from Table 3.20 in the Texas Water Board reference:

$$C_{MF} = 2.5Q_{in}$$

# **Electricity Intensity**

Electricity intensity is fixed at 0.18 kWh/m3 from Plappally & Lienhard (2012).

### References

#### **CAPITAL**

User's Manual for Integrated Treatment Train Toolbox - Potable Reuse (IT3PR) Version 2.0

Steinle-Darling, E., Salveson, A., Russel, C., He, Q., Chiu, C., Lesan, D.

Texas Water Development Board

December 2016

#### **ELECTRICITY**

Plappally, A. K. and J. H. Lienhard V (2012).

"Energy requirements for water production, treatment, end use, reclamation, and disposal." Renewable and Sustainable Energy Reviews 16(7): 4818-4848.

### **Microfiltation Module**

class watertap3.wt\_units.microfiltration.UnitProcess (\*args, \*\*kwds)

# Municipal Drinking (Distribution)

This unit is a terminal unit in WaterTAP3 and represents the initial cost to get product water to the distribution system.

#### **Unit Parameters**

None

### **Capital Costs**

The capital costs are a function of flow [MGD]:

$$C_{md} = 0.0403Q_{in}^{0.8657}$$

# **Electricity Intensity**

Electricity intensity for municipal drinking is based off the pump used. The calculation includes:

• Lift height [ft]:

h

• The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

• And the influent flow in [gal/min] and [m3/hr]:

 $Q_{gpm}, Q_{m3hr}$ 

Then the electricity intensity is calculated as:

$$E_{bw} = \frac{0.746Q_{gpm}h}{3960\eta_{pump}\eta_{motor}Q_{m3hr}}$$

# **Assumptions**

- Lift height [ft] = 300
- Pump efficiency = 0.9
- Motor efficiency = 0.9

### References

Voutchkov, N. (2018).

Desalination Project Cost Estimating and Management.

https://doi.org/10.1201/9781351242738

## Municipal Drinking (Distribution) Module

class watertap3.wt\_units.municipal\_drinking.UnitProcess (\*args, \*\*kwds)

### Ozone + AOP

The Ozone unit in WaterTAP3 is used to calculate costs for both Ozone and Ozone+AOP systems.

### **Unit Parameters**

Unit parameters are read in from the unit\_params dictionary given in the input sheet.

- "aop" boolean to indicate if the unit includes AOP costs:
  - Required parameter
  - If True, oxidant costs are included
  - If False, oxidant costs are excluded
- "contact\_time" contact time with ozone [min]
  - Required parameter
- "ct" Concentration \* time (Ct) target [mg/(L\*min)]
  - Required parameter
- "mass\_transfer" mass transfer coefficient for ozone contactor
  - Required parameter
- "chemical\_name" oxidant chemical name
  - Required parameter if aop = True
  - Must match exactly the chemical name in chemical\_name.csv

## **Capital Costs**

The Ozone/AOP unit in WaterTAP3 is used for both Ozone only units and Ozone+AOP units. For this reason costs are broken up between the ozone system and the oxidant injection system.

#### **Ozone Capital Costs**

Ozone capital costs in WaterTAP3 are a function of the ozone contact time, Ct, ozone mass transfer, ozone dose, TOC concentration, flow in, and the ozone/TOC ratio.

TOC concentration and flow in are taken from the model. Contact time, mass transfer, and Ct are taken from user input. Ozone demand is calculated from Texas Water Development Board (2016):

$$D_{O3} = \frac{t_{O3}c_{toc}Ct}{\eta_{O3}}$$

Ozone dose is then used in a regression dervied from data found in Table 3.24 from Texas Water Development Board (2016).

### **Oxidant Capital Costs**

The unit can accept any chemical name and dose, but the cost curve used was developed specifically for Hydrogen Peroxide in Texas Water Development Board (2016):

**Unit Models** 

$$C_{ox} = 1228S_{ox}^{0.2277}$$

Oxidant costs are calculated are based off the oxidant solution flow [lb/day]:

$$S_{ox} = Q_{in}D_{ox}$$

Where the oxidant dose is calculated with [kg/m3]:

$$D_{ox} = 0.5 X c_{toc}$$

And the ozone/TOC ratio X is calculated with:

$$X = 1 + \frac{t_{O3}Ct}{c_{toc}}$$

# **Electricity Intensity**

Electricity intensity is a function of the ozone flow [lb/day] and water flow into unit [m3/hr] from Mundy et al. (2018):

$$E_{O3} = 5\frac{Q_{O3}}{Q_{in}}$$

#### References

#### **COSTING**

User's Manual for Integrated Treatment Train Toolbox - Potable Reuse (IT3PR) Version 2.0

Steinle-Darling, E., Salveson, A., Russel, C., He, Q., Chiu, C., Lesan, D.

Texas Water Development Board

December 2016

# **ELECTRICITY**

Mundy, B., et al. (2018).

"A Review of Ozone Systems Costs for Municipal Applications. Report by the Municipal Committee – IOA Pan American Group."

Ozone: Science & Engineering 40(4): 266-274.

#### Ozone + AOP Module

class watertap3.wt\_units.ozone\_aop.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity for Ozone/Ozone AOP unit.

**Parameters:** ozone\_flow (float) – Flow of ozone from ozone generator [lb/day]

Returns: Ozone/Ozone AOP electricity intenstiy [kWh/m3]

#### fixed\_cap (unit\_params)

Fixed capital for Ozone/Ozone AOP unit.

#### Parameters:

- unit\_params (dict) Input parameter dictionary from input sheet
- toc\_in (float) TOC concentration into unit [mg/L]
- aop (bool) Boolean to indicate if unit is AOP or not.
- contact\_time (float) Ozone contact time [min]
- ct (float) Concentration \* time (Ct) target [mg/(L\*min)]
- mass\_transfer (float) Mass transfer coefficient
- chemical\_name (str) Name of oxidant used if unit is AOP

Returns: Fixed capital cost for Ozone/Ozone AOP [\$MM]

get\_costing (unit\_params=None, year=None)
Initialize the unit in WaterTAP3.

### solution\_vol\_flow()

Determine oxidant solution flow rate [gal/day]

Returns: Oxidant solution flow [gal/day]

### Reverse Osmosis

The capital cost, O&M costs, electricity consumption, TDS removal, and water recovery of the reverse osmosis unit model are based on a basic representation of the physical performance of the process. This includes calculations of osmostic pressure and mass balance across the membrane. The feed pressure (i.e. pump power required) and membrane area are estimated based on optimizing for LCOW, unless specified otherwise. All other variables in the reverse osmosis model have default assumptions, provided below, that factor into calculating the water recovery, TDS removal, pure water flux, and osmotic pressure.

### **Unit Parameters**

The user only has to specify whether or not to include an energy recovery device (ERD).

- "erd" whether or not to include an ERD
  - Required parameter
  - Options are "yes" or "no"

### **Unit Constraints**

The reverse osmosis unit in WaterTAP3 is broken up into a feed, permeate, and retentate IDAES Block() to track the different mass, flow, and pressure changes for each stream.

#### Mass and Pressure Constraints

The unit only uses the TDS concentration into the unit to estimate the total concentration of mass going into each reverse osmosis unit.

Thus, for each block (feed, permeate, retentate), some or all of the following mass and/or energy balance equations apply.

The total concentration of TDS flowing into the unit is [kg/m3]:

$$c_{tot} = 0.6312c_{tds} + 997.86$$

The mass concentration of water into the block is [kg/m3]:

$$c_w = c_{tot} - c_{tds}$$

The mass flow of water into the block is [kg/s]:

$$M_w = c_w Q_{in}$$

The mass flow of TDS into the block is [kg/s]:

$$M_{TDS} = c_{TDS}Q_{in}$$

The mass fraction of TDS into the block is:

$$\chi_{TDS} = \frac{M_{TDS}}{M_{W} + M_{TDS}}$$

The mass fraction of water into the block is:

$$\chi_W = \frac{M_W}{M_W + M_{TDS}}$$

The overall mass balance around water flow is:

$$M_{w,f} = M_{w,p} + M_{w,r}$$

And the overall mass balance around TDS is:

$$M_{tds,f} = M_{tds,p} + M_{tds,r}$$

#### Feed Block

The osmotic coefficient is calculated according to (Bartholomew & Mauter (2019)):

$$\sigma = 4.92x_{TDS}^2 + 0.0889x_{TDS} + 0.918$$

Then the osmotic pressure [bar] is calculated as:

$$P_{osm} = \frac{8.45 \times 10^7 \sigma x_{TDS}}{1 - x_{TDS}}$$

The flux is calculated from the feed stream as:

$$J_w = \rho_w K_w (P_{feed} - P_{atm} - 0.5P_d) - (0.5(P_{osm,f} + P_{osm,r}))$$

The pressure drop is assumed to be 3 bar.

#### Permeate Stream

The equation for mass into permeate is different than for feed or retentate streams (Bartholomew & Mauter (2019)):

$$c_{tot, p} = 756c_{tds} \times 10^{-6} + 995$$

The concentration coming out of the unit is:

$$C_{tds, out} = C_{tot, p} X_{tds, p}$$

The mass flow of water is determined from the membrane area and pure water flux:

$$M_{W,p} = J_W A$$

The mass flow of TDS is determined from the membrane area and the salt permeability coefficient:

$$M_{TDS,p} = 0.5AK_s(c_{tds,f} + c_{tds,r})$$

The pressure on the permeate side is assumed to be atmospheric:

$$P_p = P_{atm}$$

### **Capital Costs**

The capital costs for reverse osmosis has several components:

- 1. Pump capital cost
- 2. Membrane capital cost
- 3. Pressure vessel and & rack capital cost
- 4. Energy recovery device (optional)

The total capital costs for RO are calculated as follows, which each component described below:

$$C_{RO} = C_{pump} + C_{mem} + C_{erd} + 3.3C_{pv,r}$$

The value is then multiplied by the Indirect Cost Factor (IDF = 1.65) to arrive at the final fixed capital for reverse osmosis.

### **Pump Capital Costs**

The pump power is calculated as:

$$p_{pump} = \frac{Q_{in}P_f}{\eta_p}$$

The pump cost is then (Bartholomew et al., 2018):

$$C_{pump} = p_{pump} \frac{53}{10^5 \times 3600} 0.97$$

### Membrane Capital Costs

The cost per meter squared of membrane area is \$30 assumed (Bartholomew et al., 2018). The membrane costs are calculated as:

$$C_{mem} = A \times 30$$

### Pressure Vessel & Rack Capital Costs

The pressure vessel cost is a function of area and the number of vessels per membrane area (assumed to be 0.025 vessels/m2) and the vessel cost (assumed to be \$1000) based on the default EPA assumptions:

$$C_{pv} = A * 0.025$$

The rack capital costs assumes 2 trains, 150 ft start, and 5 ft per additional vessel:

$$C_{rack} = (150 + (x_{add}A0.025))33n_{trains}$$

And the total for this component is:

$$C_{pv,r} = C_{pv} + C_{rack}$$

#### **Energy Recovery Device**

The capital costs for the ERD option is taken from Bartholomew & Mauter (2019) and is based on the volumetric mass flow into the ERD device [kg/hr]:

$$M_{tot, r} = M_{H20, r} + M_{tds, r}$$

And the capital costs are calculated:

$$C_{erd} = 3134.8 M_{tot,r}^{0.58}$$

### **Electricity Intensity**

The electricity intensity is a function of the pump power, ERD power, and the flow into the unit.

The pump power is calculated as [kW]:

$$p_{pump} = \frac{Q_{in}P_f}{\eta_p}$$

The ERD power is function of the retentate flow (flow out of the unit), retentate pressure, and the ERD efficiency [kW]:

$$p_{erd} = \frac{Q_{out}(P_r - 1)}{\eta_{erd}}$$

And the electricity intensity for the unit is calculated as [kWh/m3]:

$$E_{RO} = \frac{p_{pump} - p_{erd}}{Q_{in}}$$

## Membrane Replacement Rate & Chemical Cost

The membrane replacement rate is included in the other variable operating costs for reverse osmosis.

Membrane replacement costs (assumed to be 25% of area per year):

$$C_{replace} = 0.25C_{mem}$$

Chemical costs are assumed to equal 1% of the capital cost (Bartholomew et al., 2018).

### References

Bartholomew, T. V. and Mauter, M. S. (2019).

"Computational framework for modeling membrane processes without process and solution property simplifications." *Journal of Membrane Science* 573: 682-693.

Bartholomew, T. V., Siefert, N. S., Mauter, M.S. (2018).

"Cost Optimization of Osmotically Assisted Reverse Osmosis."

Environmental Science & Technology 52: 11813-11821.

Lu, Y.-Y., et al. (2007).

"Optimum design of reverse osmosis system under different feed concentration and product specification." Journal of Membrane Science 287(2): 219-229.

US Environmental Protection Agency (2019)

"Work Breakdown Structure-Based Cost Model for Reverse Osmosis/Nanofiltration Drinking Water Treatment" https://www.epa.gov/sites/production/files/2019-07/documents/wbs-ronf-documentation-june-2019.pdf

#### Reverse Osmosis Module

class watertap3.wt\_units.reverse\_osmosis.UnitProcess (\*args, \*\*kwds)

elect (t)

**Parameters:** t (int) – Indexing variable for Pyomo Var()

Returns:

fixed\_cap (t, b\_cost)

Parameters:

• t (int) - Indexing variable for Pyomo Var()

• b\_cost (object) - Costing block for unit.

**Returns:** Fixed capital costs for reverse osmosis [\$MM]

## Sedimentation

### **Unit Parameters**

There is one parameter:

- "settling\_velocity" v the assumed settling velocity for the unit [m/s]:
  - Required parameter

# **Capital Costs**

The capital costs are a function of basin surface area:

$$C_{sed} = 13572 A_{basin}^{0.3182}$$

Basin surface area is calculated as [ft3]:

$$A_{basin} = \frac{Q_{in}}{V}$$

# **Electricity Intensity**

There are no electricity costs associated with sedimentation in WaterTAP3.

### References

William McGivney & Susumu Kawamura (2008) Cost Estimating Manual for Water Treatment Facilities DOI:10.1002/9780470260036

### Sedimentation Module

class watertap3.wt\_units.sedimentation.UnitProcess (\*args, \*\*kwds)

### Sodium Bisulfite Addition

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

### **Capital Costs**

Costing parameters for sodium bisulfite addition are taken from sulfuric acid. The sodium bisulfite solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single sodium bisulfite addition unit, a = 900.97 and b = 0.6179. The full cost equation in WaterTAP3 is:

$$C_{bisulf} = 900.97S^{0.6179}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.11 in McGivney & Kawamura (2008).

# **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

• Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{bisulf} = Q_{in}D_{bisulf}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{bisulf}}{\rho_{bisulf}}$$

• The pump and motor efficiencies:

$$\eta_{pump}$$
,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{bisulf} = \frac{0.746Sh}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

# **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1480
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

### Reference

William McGivney & Susumu Kawamura (2008) Cost Estimating Manual for Water Treatment Facilities

#### DOI:10.1002/9780470260036

#### Sodium Bisulfite Module

class watertap3.wt\_units.sodium\_bisulfite\_addition.UnitProcess (\*args, \*\*kwds)

#### elect()

Electricity intensity.

Parameters:

- lift\_height (float) Lift height for pump [ft]
- pump\_eff (float) Pump efficiency
- motor\_eff (float) Motor efficiency

**Returns:** Electricity intensity [kWh/m3]

### fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. EXAMPLE: {'dose': 10}

Fixed capital for sodium bisulfite addition is a function of sodium bisulfite dose, sodium bisulfite solution flow, and the number of units.

**Parameters:** dose (float) – Sodium bisulfite dose [mg/L]

**Returns:** Sodium bisulfite addition fixed capital cost [\$MM]

get\_costing (unit\_params=None, year=None)

Initialize the unit in WaterTAP3.

#### solution\_vol\_flow()

Chemical solution flow in gal/day

**Parameters:** solution\_density (float) – Solution density [kg/m3]

**Returns:** Sodium bisulfite solution flow [gal/day]

# Solution Distribution and Recovery Plant

The solution distribution and recovery plant distributes the irrigated solution to the stacked heap of metal-bearing ores and the recovers that solution for further extraction.

#### **Unit Parameters**

There are two parameters:

- "mining\_capacity" mining capacity for the mine [tonnes/day]
  - Optional parameter
  - Default value is 922 tonnes/day
  - Must be provided with "ore\_heap\_soln" or default values for both will be used.
- "ore\_heap\_soln" volume of leach solution needed per mass ore [gal/tonne]
  - Optional parameter
  - Default value is 500 gal/tonne
  - Must be provided with "mining\_capacity" or default values for both will be used.

### **Capital Costs**

Capital costs for the solution distribution and recovery plant and other associated mine units (i.e. Agglomeration and Stacking, Heap Leaching) are derived from Table 3 in Kappes (2002). The costing components explicitly calculated for these units via regressed data from this table are (associated WaterTAP3 unit in parentheses):

- Mining equipment (Heap Leaching)
- Mine development (Heap Leaching)
- Crushing plant (Heap Leaching)
- Leaching pads/ponds (Heap Leaching)
- Agglomeration/stacking system (Agglomeration and Stacking)
- Solution distribution and recovery plant (Solution Distribution and Recovery Plant)

The costs from this table that are estimated as a fraction of the component costs are:

- Infrastructure (power, water, access roads, site office, service facilities)
- Owner"s preproduction cost
- Engineering, procurement, construction management
- Import duties
- Equipment and materials transport
- Initial operating supplies

Note that laboratory costs and working capital costs from this table are accounted for elsewhere in WaterTAP3 and so are excluded from the unit process calculations.

Capital costs for the solution distribution and recovery plant are a function of the process pumps, plant, and solution distribution piping. These are lumped together in one costing equation that is a function of the mining capacity X [tonnes/day]. This equation is below and is derived from Table 3 in Kappes (2002):

$$C_{s\&d} = 0.00347X^{0.71917}$$

To account for the other tabulated costing components in Table 3, WaterTAP3 calculates the fraction f that the other costs are of the component costs (i.e. other costs / component costs). The other costs fraction f are determined from a regression of the total cost in Table 3 minus the solution and distribution costs (calculated above) vs. the mining capacities in that table (3,000 and 15,000 tonnes/day):

$$f = 0.3012X^{0.1119}$$

This fraction is multiplied by the cost of the process pumps, plant, and solution distribution piping (calculated above). This is the costing basis for the solution distribution and recovery plant:

$$C_{basis} = C_{s\&d}(1+f)$$

To create a cost curve based on unit flow, WaterTAP3 scales the unit flow to the recycle water flow for the solution distribution and recovery plant. The recycle water flow is the difference between the heap flow and the make up flow:

$$Q_{recycle} = Q_{heap} - Q_{makeup}$$

The make up flow and heap flow are derived from the user input for "ore\_heap\_soln" H (default is 500 gal/tonne if no user input provided) and "mining\_capacity" M (default is 922 tonnes/day if no user input provided). So making the proper unit conversions, make up flow is [m3/hr]:

$$Q_{makeup} = 0.17HM$$
  
 $Q_{heap} = HM$ 

And then the final capital costing curve for the solution distribution and recovery plant is:

$$C_{soln\&dist} = \frac{Q_{in}}{Q_{recycle}} C_{basis}^{0.71917}$$

## **Operating Costs**

The operating costs *P* [\$/year] for the solution distribution and recovery plant are derived with cost curves regressed from data in Table 5 of Kappes (2002). Included for the system distribution and recovery plant in WaterTAP3 are operational costs relating to:

- Recovery plant operations
- Site maintenance
- Cement for agglomeration
- Cyanide, lime, and other reagents
- Environmental reclamation and closure

The cost curve for all these operational costs is:

$$P_{s\&d} = 7.71759X^{0.91475} = C_{op}$$

## **Electricity Intensity**

Electricity intensity is a function of the mining capacity M and the recycle flow and is taken from Kappes (2002) and is calculated with [kWh/m3]:

$$E = \frac{1.8M}{Q_{recycle}}$$

#### References

Kappes, D.W. "Precious Metal Heap Leach Design and Practice" (2002)

in: Mineral processing plant design, practice, and control

pg. 1606-1630, ISBN: 0873352238

http://ore-max.com/pdfs/resources/precious metal heap leach design and practice.pdf

### Solution Distribution and Recovery Plant Module

class watertap3.wt\_units.solution\_distribution\_and\_recovery\_plant.UnitProcess (\*args,
\*\*kwds)

# Holding/Storage Tanks

### **Unit Parameters**

- $\bullet$  "avg\_storage\_time" storage time for volume calculation [hr]
  - Required parameter
- "surge\_cap" desired surge capacity for volume calculation
  - Required parameter
  - · Can be zero if no surge capacity is desired

## **Capital Costs**

Storage tank capital costs are calculated as a function of the volume of storage [m3] required V, flow in [m3/hr], storage duration t [hr], and surge capacity needed x:

$$V = Q_{in}t(1+x)$$

The storage volume is used to calculate capital costs (\$MM):

$$C_{tank} = 1.48 \times 10^{-4} V^{1.014}$$

The data to make the regression is from Loh et al. (2002).

## **Electricity Intensity**

There are no electricity costs associated with storage tanks in WaterTAP3.

#### Reference

Loh, H. P., Lyons, J., White, C.W. (2002)

DOE/NETL-2002/1169 - Process Equipment Cost Estimation Final Report.

United States: N. p., 2002. Web. doi:10.2172/797810.

https://www.osti.gov/servlets/purl/797810

## Storage Tank Module

class watertap3.wt\_units.holding\_tank.UnitProcess (\*args, \*\*kwds)

### elect()

WaterTAP3 has no electricity intensity associated with storage tanks.

fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. EXAMPLE: {'avg\_storage\_time': 24, 'surge\_cap': 0.2}

Parameters:

- avg\_storage\_time storage time in hours
- surge\_cap is the surge capacity used for calculating storage volume, expressed as a fraction of the total flow (e.g. for 20% surge capacity, use 0.2)

Returns: Fixed capital for storage tanks.

## Sulfuric Acid Addition

Costs for chemical additions are based on the chemical dose required to treat the water and the inlet flow to the unit.

### **Unit Parameters**

There is one unit parameter:

- "dose" dose of chemical [mg/L]
  - Required parameter

## **Capital Costs**

The sulfuric acid solution flow S [gal/day] is used in a cost curve of the general form:

$$C = aS^b$$

For a single sulfuric acid addition unit, a = 900.97 and b = 0.6179. The full cost equation in WaterTAP3 is:

$$C_{sulf} = 900.975^{0.6179}$$

This cost is then multiplied by the number of units and the EIF factor for the final FCI for the chemical addition. These parameters were determined by fitting data from Figure 5.5.11 in McGivney & Kawamura (2008).

## **Electricity Intensity**

Electricity intensity for chemical additions is based off the pump used to inject the chemical solution, the chemical solution flow rate, and the influent flow rate. The calculation includes:

Lift height [ft]:

h

• The mass flow rate [kg/day] of the solution necessary to achieve the desired dose:

$$M_{sulf} = Q_{in}D_{sulf}$$

• The volumetric flow S [gal/min] of the chemical solution, which incorporates the solution density [kg/m3]:

$$S = \frac{M_{sulf}}{\rho_{sulf}}$$

• The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

Then the electricity intensity is calculated as [kWh/m3]:

$$E_{sulf} = \frac{0.7465h}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

## **Assumptions**

- Number of units = 2
- Solution density [kg/m3] = 1781
- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

### Reference

William McGivney & Susumu Kawamura (2008) Cost Estimating Manual for Water Treatment Facilities DOI:10.1002/9780470260036

### Sulfuric Acid Addition Module

```
class watertap3.wt_units.sulfuric_acid_addition.UnitProcess (*args, **kwds)
  elect()
    Electricity intensity.
         Parameters:
                           • lift_height (float) - Lift height for pump [ft]
                           • pump_eff (float) - Pump efficiency
                           • motor eff (float) - Motor efficiency
            Returns:
                       Electricity intensity [kWh/m3]
  fixed_cap (unit_params)
    "unit_params" are the unit parameters passed to the model from the input sheet as a Python dictionary.
    EXAMPLE: {'dose': 10}
            Returns: Sulfuric acid addition fixed capital cost [$MM]
  get_costing (unit_params=None, year=None)
    Initialize the unit in WaterTAP3.
  solution_vol_flow()
    Chemical solution flow in gal/day
         Parameters: solution_density (float) – Solution density [kg/m3]
                       Sulfuric acid solution flow [gal/day]
```

# Surface Discharge

### **Unit Basics**

This unit is a terminal unit in WaterTAP3 and represents the cost of discharging waste streams to surface water. This is also the assumed destination for the waste from any unit process if no waste steram is specified in the input sheet.

## **Unit Parameters**

There are two parameters:

- "pipe\_distance" distance for piping to discharge to surface water body [mi]:
  - Optional parameter
  - If included in parameters, adds pipe construction cost to capital cost.
- "pump" whether or not to include pumping electricity costs:
  - Optional parameter
  - Options are "yes" and "no"
  - If "yes", includes electricity calculation.

## **Capital Costs**

The capital costs are a function of flow [m3/hr] and can include piping costs:

$$C_{surf} = 35 \frac{Q_{in}}{10417} 0.873 + C_{pipe}$$

Piping cost assumes an 8 in diameter pipe, and is calculated as:

$$C_{pipe} = 0.28x_{pipe}$$

If the "pipe\_distance" unit parameter is not included:

$$C_{pipe} = 0$$

## **Electricity Intensity**

Electricity intensity for surface discharge (if included) is based off the pump used. The calculation includes:

• Lift height [ft]:

h

• The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

• And the influent flow in [gal/min] and [m3/hr]:

$$Q_{apm}, Q_{m3hr}$$

Then the electricity intensity is calculated as:

**Unit Models** 

$$E_{surf} = \frac{0.746Q_{gpm}h}{3960\eta_{pump}\eta_{motor}Q_{m3hr}}$$

# **Assumptions**

- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

## References

# Surface Discharge Module

class watertap3.wt\_units.surface\_discharge.UnitProcess (\*args, \*\*kwds)

## Seawater Intake

This is the intake unit process for seawater cases.

## **Unit Parameters**

None.

## **Capital Costs**

The capital costs are a function of flow [MGD] are from Voutchkov (2018):

$$C_{sw} = 2.15 \times 10^{-4} Q_{in}^{0.888803}$$

## **Electricity Intensity**

Electricity intensity for seawater intake is based off the pump used. The calculation includes:

• Lift height [ft]:

h

The pump and motor efficiencies:

 $\eta_{pump}$ ,  $\eta_{motor}$ 

• And the influent flow in [gal/min] and [m3/hr]:

 $Q_{gpm}$ ,  $Q_{m3hr}$ 

Then the electricity intensity is calculated as:

$$E_{sw} = \frac{0.746Q_{gpm}h}{3960\eta_{pump}\eta_{motor}Q_{m3hr}}$$

## **Assumptions**

- Lift height [ft] = 100
- Pump efficiency = 0.9
- Motor efficiency = 0.9

#### References

Voutchkov, N. (2018).

Desalination Project Cost Estimating and Management.

https://doi.org/10.1201/9781351242738

## Seawater Intake Module

class watertap3.wt\_units.sw\_onshore\_intake.UnitProcess (\*args, \*\*kwds)

## Tri-Media Filtration

### **Unit Parameters**

None

## **Capital Costs**

The capital costs are a function of flow [MGD] from the Texas Water Development Board (2016):

 $C_{tri} = 0.72557Q_{in}^{0.5862}$ 

## **Electricity Intensity**

Electricity intensity is fixed at 0.00045 kWh/m3 from Bukhary et al. (2019).

### References

#### **CAPITAL**

User's Manual for Integrated Treatment Train Toolbox - Potable Reuse (IT3PR) Version 2.0

Steinle-Darling, E., Salveson, A., Russel, C., He, Q., Chiu, C., Lesan, D.

**Texas Water Development Board** 

December 2016

### **ELECTRICITY**

Bukhary, S., et al. (2019).

"An Analysis of Energy Consumption and the Use of Renewables for a Small Drinking Water Treatment Plant." Water 12(1).

### Tri-Media Filtration Module

class watertap3.wt\_units.tri\_media\_filtration.UnitProcess (\*args, \*\*kwds)

## UV + AOP

The UV+AOP module is used to determine costs for both UV disinfection and UV + AOP units.

Capital costs for UV systems in WaterTAP3 are significantly influenced by UV Dose, UVT, and flow. For most accurate capital cost, include facility data with input parameters.

#### Unit Parameters

This module has one required parameter and three optional parameters for the input sheet:

- "aop" boolean indicating if unit includes AOP or not:
  - Required parameter
  - If True, include chemical costs
- "uvt\_in" assumed ultraviolet transmittance (UVT) into unit:
  - Optional parameter
  - Default value is 0.9
  - Must be between 0.5 and 0.99 in increments of 0.01
- "uv\_dose" Reduction Equivalent Dose (RED) for unit:
  - Optional parameter
  - Default value is 100 mJ/cm2
  - Must be <1200 in increments of 10
- "chemical\_name" name of chemical used for oxidant:
  - Optional parameter
  - No default value
  - Can be any chemical but must match *exactly* chemical entry in catalysts\_chemicals.csv, e.g. "Hydrogen\_Peroxide"

## Capital Costs

Capital costs for UV + AOP includes cost for the UV system and for the oxidant injection system:

$$C_{UV+AOP} = C_{UV} + C_{ox}$$

## **UV Capital Costs**

Capital costs are a function of flow, UV dose, and UV Transmission (UVT). The WaterTAP3 model uses data Table 3.22 in Texas Water Development Board (2016) to interpolate cost values for:

- UVT between 0.5 and 0.99 in increments of 0.01.
- UV Dose between 10 and 1,200 mJ/cm2 in increments of 10.

For the given UVT and UV Dose, WaterTAP3 retrieves cost data for flows between 1 and 25 MGD from data/uv\_cost\_interp.csv. Using this data, a cost curve is fit to a power curve. Once a and b are known, capital costs for the UV system are determined:

$$C_{UV} = aQ_{in}^b$$

#### **Oxidant Capital Costs**

The unit can accept any chemical name and dose, but the cost curve used was developed specifically for Hydrogen Peroxide.

Oxidant costs are calculated with:

$$C_{ox} = 1228(Q_{in}D_{ox})^{0.2277}$$

Where the oxidant dose [kg/m3] is taken from the input parameter "dose".

If "aop" is False in the unit parameters:

$$C_{ox} = 0$$

## **Electricity Intensity**

Electricity intensity for UV/AOP is fixed at 0.1 kWh/m3 and is taken from USEPA (2010).

#### References

#### CAPITAL

User's Manual for Integrated Treatment Train Toolbox - Potable Reuse (IT3PR) Version 2.0 Steinle-Darling, E., Salveson, A., Russel, C., He, Q., Chiu, C., Lesan, D. **Texas Water Development Board** 

December 2016

#### **ELECTRICITY**

US Environmental Protection Agency (2010)

"Evaluation of Energy Conservation Measures for Wastewater Treatment Facilities" https://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P1008SBM.TXT

## UV + AOP Module

class watertap3.wt\_units.uv\_aop.UnitProcess (\*args, \*\*kwds)

fixed\_cap (unit\_params)

"unit\_params" are the unit parameters passed to the model from the input sheet as a Python dictionary. EXAMPLE: {'aop': True, 'uv\_dose': 350, 'dose': 5, 'chemical\_name': 'Hydrogen Peroxide'}

#### Parameters:

- aop (bool) (required) Boolean that determines if UV is used with AOP. Must be either True or False
- uvt in (float) (optional, default is 0.9) UV transmission (UVT) into unit
- uv\_dose (float) (optional, default is 100) Reduction Equivalent Dose (RED) [mJ/cm2]
- dose (float) (optional, no default) Dose for oxidant (if AOP) [mg/L]
- chemical\_name (str) (optional, default is 'Hydrogen\_Peroxide') Name of oxidant used for AOP.

Returns: Fixed capital for UV or UV+AOP unit [\$MM]

```
get_costing (unit_params=None, year=None)
Initialize the unit in WaterTAP3.
```

## solution\_vol\_flow()

Determine oxidant solution flow rate in gal / day

Returns: Oxidant solution flow [gal/day]

### uv\_regress()

Determine a, b costing parameters as a function of flow, UVT, and UV dose for unit.

### Parameters:

- flow\_in (float) Volumetric flow into unit [MGD]
- uvt\_in (float) UV transmission (UVT) into unit
- uv\_dose (float) UV dose used by the unit [mg/L]

Returns: a, b

# Water Pumping Station

#### **Unit Basics**

This is a pump unit in WaterTAP3.

## **Unit Parameters**

There are three unit parameters:

- "pump\_type" the type of water pumping station:
  - Required parameter
  - Options are "raw" or "treated"
  - Different costing values are used for each option
- "pump\_power" pump power if available [hp]:
  - Optional parameter
- "lift\_height" amount of dynamic head [ft]:
  - Optional parameter
  - Default value is 100 ft

# **Capital Costs**

Depending on the value for "pump\_type", different cost curves are used for the general form with flow in [MGD] from McGivney & Kawamura (2008):

$$C_{wps} = aQ_{in}^b$$

For "pump\_type" = "raw":

- a = 19370.36
- b = 0.9149

For "pump\_type" = "treated":

- a = 40073.43
- b = 0.8667

## **Electricity Intensity**

If there is no input for "pump\_power", electricity intensity is a function of flow [gpm] and the unit parameter "lift\_height" h:

$$E_{wps} = \frac{0.746Q_{gpm}h}{3960\eta_{pump}\eta_{motor}Q_{in}}$$

With assumed pump and motor efficiencies of 90%.

Otherwise, the input for "pump\_power" is converted from horsepower to kW and electricity intensity is:

$$E_{wps} = \frac{p_{pump}}{Q_{in}}$$

## References

William McGivney & Susumu Kawamura (2008) Cost Estimating Manual for Water Treatment Facilities DOI:10.1002/9780470260036

# Water Pumping Station Module

class watertap3.wt\_units.water\_pumping\_station.UnitProcess (\*args, \*\*kwds)

## Well Field

### **Unit Parameters**

There are two unit parameters:

- "pipe\_distance" pipe distance to be included in costing model [miles]
  - Optional parameter
  - If not provided, piping cost is not included in cost model
  - Cost is \$280,000 per mile assuming an 8 in pipe
- "pump" to include pumping costs
  - Optional parameter
  - Options are "yes" or "no"
  - Default value is "yes"

## **Capital Costs**

The capital costs are a function of flow [m3/hr] from Voutchkov (2018). If a pipe distance is not provided, the capital costs are:

$$C_{wf} = 4731.6Q_{in}^{0.9196}$$

If pipe distance *d* is provided, the piping cost is:

$$C_{pipe} = 280000d$$

And the total cost then would be:

$$C_{tot} = C_{wf} + C_{pipe}$$

## **Electricity Intensity**

There are no electricity costs associated with well field in WaterTAP3.

#### References

Voutchkov, N. (2018).

Desalination Project Cost Estimating and Management.

https://doi.org/10.1201/9781351242738

## Well Field Module

class watertap3.wt\_units.well\_field.UnitProcess (\*args, \*\*kwds)

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