**Air Stripping Pre- and Post-Treatment Model (0D):**

**Prepared for the NREL “Pathways to Achieving Pipe Parity for Solar Thermal Desalination of High Salinity Brines” project.**

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**This is an Air Stripping model that works under the following criteria and assumptions:**

* Supports a single liquid phase only.
* Supports the adsorption of a single solute species only while other species are considered inert.
* Supports steady state only.
* Assumes isothermal conditions.
* Assumes isobaric conditions.

**Introduction**

Air stripping is defined as a process whereby volatile constituents such as gases and organic compounds are transferred from the water to the air. An air stripping approach involves the use of packed towers or countercurrent flow towers, normally known as gas-phase contactors, have a continuous gas phase and a discontinuous water phase and are typically used to remove (or strip) gases or volatile organic chemicals (VOCs) from water. Packed towers are the most used and these are circular or square towers that are filled with an irregular shaped inert packing material, as shown in Figure 1.

Diagram of a liquid distribution system

Description automatically generated with low confidence

Figure 1: Schematic of a countercurrent packed tower.

Packing material is available in a wide variety of sizes and shapes depending on the manufacturer. Operationally, water is pumped to the top of the tower and into a liquid distributor where it is dispersed as uniformly as possible across the packing surface, and then it flows by gravity through the packing material and is collected at the bottom of the tower. Airflow may be in the same direction as the water (co-current), in the opposite direction as the water (countercurrent), or across the water (cross flow). For countercurrent operation, a blower is used to introduce fresh air into the bottom of the tower and the air flows countercurrent to the water up through the void spaces between the wetted packing material. The model design is based on a countercurrent packed tower operation.

**Degrees of Freedom (DOF)**

The Air Stripping (0D) model has at least 18 degrees of freedom that the user must specify. The table below gives an outline of these:

Table 1: Air Stripping Model - Degrees of Freedom

|  |  |  |
| --- | --- | --- |
| **Description** | **Model Variable Name** | **Units** |
| Influent concentration  of target pollutant | Ci | mg/L |
| Liquid flowrate | Ql | m3/s |
| Gas to water ratio | Gas\_to\_liq\_ratio | dimensionless |
| Liquid temperature | Tl\_K | Kelvin |
| Gas temperature | Tg\_K | Kelvin |
| Liquid density | dens\_liq | kg/m3 |
| Liquid viscosity | visc\_liq | kg/m-s |
| Gas density | dens\_gas | kg/m3 |
| Gas viscosity | visc\_gas | kg/m-s |
| Henry’s constant1 | Ht | dimensionless |
| Overall mass transfer coefficient2 | kla | s-1 |
| Pressure drop3 | P\_drop | Pascal/m |
| Packing material | ‘plastic’, ‘ceramic’, or ‘metal’ | - |
| Packing factor3 | pack\_fact | dimensionless |
| Port diameter4 | Diameter\_port | inches |
| Pipe diameter4 | Diameter\_pipes | inches |
| Pump efficiency4 | Eff\_pump | dimensionless |
| Blower efficiency4 | Eff\_blow | dimensionless |

1. The user can provide his own Henry’s constant. It’s recommended that the user considers the temperature and ionic strength of the liquid being treated when considering the selection of the constant.
2. The overall mass transfer coefficient can be determined for a specific chemical through pilot studies.
3. The pressure drop can be in the range of 45 to 1,200 Pascals per meters. These can be supplied by the packing manufacturer.
4. The pipe and port diameter for the liquid and gas input in the system can both be set to the default (6 inches). The same goes for the efficiency of the pump and blower, 85% and 40%, respectively.

The following input variables are required when specific configuration options are selected.

If *Henrys\_const* is set to "calculated":

Table 2: Required model inputs for Henry’s constant adjustment.

|  |  |  |
| --- | --- | --- |
| **Description** | **Model Variable Name** | **Units** |
| Henry’s constant of  the target pollutant at 25 °C | H | dimensionless |
| The octanol-water partition coefficient of the target pollutant | logKOW | dimensionless |
| The liquid’s ionic strength | Ionic | M (mol/L) |
| The standard enthalpies change of dissolution in water at 25 °C | Enthalpies | kJ/mol |

If *mass\_transfer\_coeff\_kla* is set to "*calculated*":

Table 3: Required model inputs for mass transfer coefficient calculation.

|  |  |  |
| --- | --- | --- |
| **Description** | **Model Variable Name** | **Units** |
| Critical volume of target pollutant | Critic\_vol | cm3/mol |
| Molecular weight of target pollutant | MWchem | g/mol |
| Normal boiling point of target pollutant | T\_norm\_boiling | Kelvin |
| Specific surface area of packing | pack\_surface\_area | 1/m |
| Nominal packing diameter | pack\_diam | m |
| Critical surface tension of packing | Stc | kg/s2 |

If *air\_to\_water\_ratio* is set to "*calculated*":

Table 4: Required model inputs for the air to water ratio calculation.

|  |  |  |
| --- | --- | --- |
| **Description** | **Model Variable Name** | **Units** |
| Target effluent of the pollutant | Ce | mg/L |

**Additional notes:**

* The U.S. EPA designated air stripping and granular-activated carbon (GAC) as best available technology (BAT) for treatment of VOCs except for vinyl chloride and methylene chloride. For these two chemicals, only air stripping is recognized as BAT.
* Typical packed tower heights usually do not exceed about 9 m (30 ft). Should the calculated tower length exceed 9 m, the air-to-water ratio could be increased by increasing the air flow rate to achieve the same treatment objective but with a smaller tower height (Edzwald, 2011).

**Case Studies for Validation:**

Case Study 1 (Edzwald, 2011):

Case Study Data:

* Liquid = Water
* Gas = Air
* **Target** chemical = 1,1,1-Trichloroethane (TCA)
* Influent = 165 µg/L = 0.165 mg/L
* **Target** effluent = 5 µg/L = 0.005 mg/L
* TDS = 1,000 mg/L as NaCl (Assumption)
* Liquidflow = 0.158 m3/s (3.6 MGD)
* Liquid temperature = 15 °C
* Gas temperature = 15 °C
* Ambient pressure = 1 atm = 101,325 Pa
* MW of target chemical = 133.4 g/mol
* Henry’s constant (dimensionless) at 15 °C = 0.487
* Molar volume at boiling point = 109 cm3/mole
* Normal boiling point temperature = 74.1 °C
* Liquid density at 15 °C = 999.15 kg/ m3
* Gas density at 15 °C = 1.22 kg/ m3
* Liquid viscosity at 15 °C = 0.00115 kg/ m - s
* Gas viscosity at 15 °C = 0.0000175 kg/ m - s
* Packing characteristics:
  + Type = Plastic
  + Nominal diameter = 0.0889 m
  + Nominal surface area = 242 m2/m3
  + Critical packing surface tension = 0.033 N/m
  + Packing factor = 33
* Pressure drop = 75 Pa/m
* Blower efficiency = 40%
* Pump efficiency = 85%

Table 5: Case study one comparison

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | **Case Study** Value1 | **Model** Outputs | % Difference  case study vs model |
| Liquid surface tension | 0.0735 N/m | 0.07348 N/m | 0.027% |
| Henry’s const. (25 °C) | - | 0.712 | - |
| Henry’s const. (Salinity) | - | 0.715 | - |
| Henry’s const. (15 °C) | 0.487 | 0.485 | 0.411% |
| Minimum air-water ratio | 2 | 1.998 | 0.100% |
| Optimal air-water ratio | 7 | 6.99 | 0.142% |
| Stripping Factor | - | 3.39 | - |
| Pressure-drop variable M | 0.0015 | 0.0015409 | 3.214% |
| Air mass loading rate | 0.335 kg/m2-s | 0.334 kg/m2-s | 0.298% |
| Water mass loading rate | 39.2 kg/m2-s | 39.171 kg/m2-s | 0.074% |
| Gas flow | 1.10 m3/s | 1.10 m3/s | 0% |
| Area | 4 m2 | 4.03 m2 | 0.747% |
| Diameter | 2.26 m | 2.265 m | 0.221% |
| Molar volume at  boiling point | 109 cm3/mole | 110.07 cm3/mole | 0.9132% |
| Liquid diffusion coefficient | 7.13 E-10 m2/s | 7.09 E-10 m2/s | 0.562% |
| Gas diffusion | 8.03 E-6 m2/s | 7.944 E-6 m2/s | 1.076% |
| Liquid-phase  mass transfer coefficient | 2.76 E-4 m/s | 3.646 E-4 m/s | 27.66% |
| Gas-phase mass transfer coefficient | 5.09E-4 m/s | 5.632 E-4 m/s | 10.11% |
| Specific surface area | 150 m2/m3 | 147.6 m2/m3 | 1.626% |
| Overall mass transfer coefficient | 0.0189 s-1 | 0.0161 s-1 | 16% |
| HTU | - | 2.43 m |  |
| NTU | - | 4.48 |  |
| Packing height | 8 m | 10.88 m | 30.50% |
| Tower height | - | 13.05 m |  |
| Pressure losses | 20.8 Pa | 20.667 Pa | 0.641% |
| Total pressure in | 101,948 Pa | 102,324.86 Pa | 0.368% |
| Blower power | 1.7 kW | 2.741 kW | 46.82% |
| Pump power | 17 kW | 23.787 kW | 33.25% |
| CAPEX | - | $754,218.12 | - |
| OPEX | - | $270,171.29 /yr | - |

Case Study 2 (Crittenden, 2012):

Case Study Data:

* Liquid = Water
* Gas = Air
* **Target** chemical = o-Dichloropropane (DCP)
* Influent = 1 mg/L
* **Target** effluent = 0.1 mg/L
* TDS = 100 mg/L as NaCl (Assumption)
* Liquidflow = 0.1 m3/s (2.28 MGD)
* Liquid temperature = 10 °C
* Gas temperature = 10 °C
* Ambient pressure = 1 atm = 101,325 Pa
* MW of target chemical = 112.98 g/mol
* Henry’s constant (dimensionless) at 10 °C = 0.0525
* Liquid density at 10 °C = 999.7 kg/ m3
* Gas density at 10 °C = 1.247 kg/ m3
* Liquid viscosity at 10 °C = 0.001307 kg/ m - s
* Gas viscosity at 10 °C = 0.0000179 kg/ m - s
* Packing characteristics:
  + Type = Plastic
  + Nominal diameter = 0.0889 m
  + Nominal surface area = 125 m2/m3
  + Critical packing surface tension = 0.033 N/m
  + Packing factor = 39
* Pressure drop = 50 Pa/m
* Blower efficiency = 35%
* Pump efficiency = 80%

Table 6: Case study two comparison

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | **Case Study** Value1 | **Model** Outputs | % Difference  case study vs model |
| Liquid surface tension | 0.0742 N/m | 0.0742 N/m | - |
| Henry’s const. (25 °C) | - | 0.146 | - |
| Henry’s const. (Salinity) | - | 0.146 | - |
| Henry’s const. (10 °C) | 0.0525 | 0.075 | 35.29% |
| Minimum air-water ratio | 17.14 | 11.95 | 35.60% |
| Optimal air-water ratio | 60 | 41.83 | 35.57% |
| Stripping Factor | 3.15 | 3.15 | 0% |
| Pressure-drop variable M | 0.005 | 0.00437 | 13.44% |
| Air mass loading rate | 1.01 kg/m2-s | 0.521 kg/m2-s | 63.87% |
| Water mass loading rate | 13.5 kg/m2-s | 10.12 kg/m2-s | 27.75% |
| Gas flow | 6 m3/s | 4.12 m3/s | 37.15% |
| Area | 7.4 m2 | 9.97 m2 | 28.60% |
| Diameter | 3.07 m | 3.565 m | 14.38% |
| Liquid diffusion coefficient | 6.08 E-10 m2/s | 6.13 E-10 m2/s | 0.819% |
| Gas diffusion | 7.65 E-6 m2/s | 7.68 E-6 m2/s | 0.391% |
| Liquid-phase  mass transfer coefficient | 1.95 E-4 m/s | 1.70 E-4 m/s | 13.69% |
| Gas-phase mass transfer coefficient | 3.63 E-3 m/s | 2.27 E-3 m/s | 46.10% |
| Specific surface area | 67 m2/m3 | 61.2 m2/m3 | 8.72% |
| Overall mass transfer coefficient | 0.00452 s-1 | 0.00365 s-1 | 12.45% |
| HTU | 3.04 m | 0.578 m | 136% |
| NTU | 2.57 | 2.881 | 11.37% |
| Packing height | 7.8 m | 1.665 m | 129.6% |
| Tower height | - | 2 m | - |
| Pressure losses | 186 Pa | 48.34 Pa | 117.94% |
| Total pressure in | 101,894 Pa | 101,473 Pa | 0.081% |
| Blower power | 9.56 kW | 1.5 kW | 145.7% |
| Pump power | 9.73 kW | 2.3 kW | 123.5% |
| CAPEX | - | $614,459.92 | - |
| OPEX | - | $204,118.88/yr | - |

***Note*:**

The high difference percentages in this case study are due to the differences in Henry’s constant prediction (35%) compared to the specified one in (Crittenden, 2012) and the difference in the calculation process of the air mass loading rate presented in (Crittenden, 2012). The calculation in (Crittenden, 2012) uses a conversion value (3.28) in the packing factor on the air mass loading rate equation. The coefficient 3.28 is a conversion factor when the packing factor in SI units (m−1) is used because the Eckert diagram was originally drawn in English units. The inclusion of this coefficient in the air mass loading rate equation affects the calculation. This coefficient is observed in the air mass loading rate equation presented in (Crittenden, 2012), while in others it is not used (Edzwald, 2011; Mackenzie L. Davis, 2010; Mines, 2014). When the air mass loading rate model equation is altered to be similar to the one presented in (Crittenden, 2012) along with some slight modifications in other constraints to attain to this example, and the correct Henry’s constant is inputted into the model rather than calculated, the results are much more in tune to the values in case study two (Table 7).

**Re-validation of this case was done by:**

* Specifying the Henry’s constant, hence specifying it in the model rather than making the system adjust it (Henrys\_const = **None**).
* **IF** air\_to\_water\_ratio configuration is not specified as “calculated” the Ce constraint, else the Ce target needs to be specified (0.1 mg/L):
* constraint\_scaling\_transform 🡪(m.Ce\_constr,1E-12)
* Altering the gas mass loading equation by dividing the variable Cf by 3.28:

m.MassLoad\_gas\_constr = Constraint(expr=m.MassLoad\_gas == sqrt((m.Press\_drop\_M \* m.dens\_gas \* (m.dens\_liq-m.dens\_gas))/((m.Cf)\*(m.visc\_liq\*\*0.1))))

m.MassLoad\_gas\_constr = Constraint(expr=m.MassLoad\_gas == sqrt((m.Press\_drop\_M \* m.dens\_gas \* (m.dens\_liq-m.dens\_gas))/((m.Cf**/3.28**)\*(m.visc\_liq\*\*0.1))))

* Convert some constraints into expressions due to scaling issues….
* #m.Load\_liq\_constr = Constraint(expr=m.Load\_liq == m.Ql/m.A\_cross)

m.Load\_liq = **Expression**(expr= m.Ql/m.A\_cross)

#m.kla\_constr  = Constraint(expr=m.kla == 0.7\*(1/(((1/(m.kl\*m.wet\_area\_pack)) + (1/(m.kg\*m.wet\_area\_pack\*m.Ht)))))) m.kla  = **Expression**(expr=0.7\*(1/(((1/(m.kl\*m.wet\_area\_pack)) + (1/(m.kg\*m.wet\_area\_pack\*m.Ht))))))

Table 7: Case study two comparison with equation modification for testing

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | **Case Study** Value1 | **Model** Outputs | % Difference  case study vs model |
| Liquid surface tension | 0.0742 N/m | 0.0742 N/m | - |
| Henry’s const. (25 °C) | - | - | - |
| Henry’s const. (Salinity) | - | - | - |
| Henry’s const. (10 °C) | 0.0525 | 0.0525 (Input) | 0% |
| Minimum air-water ratio | 17.14 | 17.143 | 0.0175% |
| Optimal air-water ratio | 60 | 60 | 0% |
| Stripping Factor | 3.15 | 3.15 | 0% |
| Pressure-drop variable M | 0.005 | 0.00535 | 6.76% |
| Air mass loading rate | 1.01 kg/m2-s | 1.044 kg/m2-s | 3.31% |
| Water mass loading rate | 13.5 kg/m2-s | 13.97 kg/m2-s | 3.42% |
| Gas flow | 6 m3/s | 6 m3/s | 0% |
| Area | 7.4 m2 | 7.168 m2 | 3.18% |
| Diameter | 3.07 m | 3.02 m | 1.64% |
| Liquid diffusion coefficient | 6.08 E-10 m2/s | 6.12 E-10 m2/s | 0.655% |
| Gas diffusion | 7.65 E-6 m2/s | 7.68 E-6 m2/s | 0.391% |
| Liquid-phase  mass transfer coefficient | 1.95 E-4 m/s | 1.99E-4 m/s | 2.03% |
| Gas-phase mass transfer coefficient | 3.63 E-3 m/s | 3.69 E-3 m/s | 1.63% |
| Specific surface area | 67 m2/m3 | 67 m2/m3 | 0% |
| Overall mass transfer coefficient | 0.00452 s-1 | 0.00460 s-1 | 1.75% |
| HTU | 3.04 m | 3.03 m | 0.329% |
| NTU | 2.57 | 2.88 | 11.37% |
| Packing height | 7.8 m | 8.72 m | 11.13% |
| Tower height | - | 10.46 m | - |
| Pressure losses | 186 Pa | 192 Pa | 3.17% |
| Total pressure in | 101,894 Pa | 102,040.88 Pa | 0.144% |
| Blower power | 9.56 kW | 12.24 kW | 24.58% |
| Pump power | 9.73 kW | 12.82 kW | 27.40% |
| CAPEX | - | $ 1,067,437.05 | - |
| OPEX | - | $ 223,748.17 /yr | - |

*\* The main issue with this validation comes from the approach presented in (Crittenden, 2012) being incorrect.*

*\* Scaling issues with the model remain, and when constraints are scaled it miscalculates the value that it is supposed to give.*

**Default chemical values based on literature (Crittenden, 2012; Edzwald, 2011):**

Table 8: Default values for chemicals available in model

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Chemical** | **H (25°C)1** | **MW2** | **Vc3** | **ΔH°dis4** | **Log Kow5** | **Tboiling6** |
| Benzene | 0.216 | 78.11 | 256 | 28.1 | 2.13 | 353.2 |
| Ethylbenzene | 0.322 | 106.17 | 374 | 39.4 | 3.15 | 409.1 |
| Chlorobenzene | 0.147 | 112.56 | 303 | 30.6 | 2.84 | 405.1 |
| Propylbenzene | 0.442 | 120.20 | 441 | 36.4 | 3.69 | 432.2 |
| o-Dichlorobenzene | 0.064 | 147 | 360 | 37.3 | 3.38 | 453.3 |
| m-Dichlorobenzene | 0.117 | 147 | 359 | 35.3 | 3.53 | 446.1 |
| p-Dichlorobenzene | 0.130 | 147 | 364 | 28.4 | 3.44 | 447.1 |
| Toluene | 0.263 | 92.14 | 316 | 32.4 | 2.73 | 383.7 |
| Carbon Tetrachloride | 1.210 | 153.82 | 276 | 33.0 | 2.83 | 349.9 |
| o-Dichloropropane | 0.146 | 112.98 | 226 | 31.1 | 1.98 | 369.1 |
| m-Xylene | 0.304 | 106.16 | 376 | 38.6 | 3.20 | 412.1 |
| o-Xylene | 0.199 | 106.16 | 369 | 31.3 | 3.12 | 417.5 |
| p-Xylene | 0.304 | 106.16 | 379 | 34.8 | 3.15 | 411.5 |
| Chloroform | 0.172 | 119.38 | 239 | 33.5 | 1.97 | 334.3 |
| 1,1,1-Trichloroethane | 0.712 | 133.4 | 294 | 28.7 | 2.49 | 347.1 |
| Methane | 28.41 | 16.04 | 98 | 14.8 | 1.09 | 111.5 |
| Carbon dioxide | 1.1 | 44.01 | 94 | 19.9 | 0.83 | 194.7 |
| Ammonia | 0.0006 | 17.03 | 73 | 36.1 | 0.23 | 239.8 |

1. Dimensionless Henry’s constant at 25°C (298.15 K)🡪 Units = Liters of Water / Liter of Gas
2. Molecular weight of the VOC compound in g/mol.
3. Critical molar volumes of different VOC’s in cm3 per mol. Adapted from trustworthy chemical information sources.
4. Standard enthalpies change of dissolution in water in kJ/mol at 25°C (298.15 K). Values were adapted from experimental dataset from (<https://pubs.acs.org/doi/pdf/10.1021/es050527h>)
5. The Octanol/Water Partition Coefficient (log Kow) are adapted from online chemical information sources.
6. Boiling temperature of chemical in Kelvin, adapted from online chemical information sources.

**Adjustments for Henry’s constants**

Temperature effect on dimensionless H:

Use of van’t Hoff equation based on (Crittenden, 2012; Edzwald, 2011):

Where:

Ionic strength effect on the apparent H:

Gases or synthetic organic chemicals (SOCs) have a higher apparent dimensionless Henry’s law constant when the dissolved solids are high because equilibrium depends on activity, not concentration (Crittenden, 2012).

The activity coefficient is calculated as:

*The values of Ks need to be determined experimentally because there is no general theory for predicting them. Salting-out coefficients for several compounds in seawater are available in the literature (Gossett, 1987;Schwarzenbach et al., 1993).* *Significant increases in volatility and the apparent Henry’s constant are only observed for high ionic strength waters, such as seawater.*

The salting out (Setschenow) coefficient can be approximated with equations reported in (Burant, 2015) and have also documented almost all available NaCl Setschenow coefficients for multiple VOC’s. They developed two approaches to determine the salting out coefficient. Approach one consists in the use of octanol/water partition coefficient (log Kow), while approach two consists in the use of much more complex experimental constants such as the Abraham solvation parameters (ASPs). ASPs account for size and intermolecular interactions, such as van der Waals forces and hydrogen bonding interactions. For the sake of simplicity and due to the high quantity of reported values for different VOC’s, the octanol/water partition coefficient approach is selected. The salting-out coefficient is focused on salinity in the form of NaCl. Yet, it must be noted that the log Kow approach exhibited larger errors in comparison with the ASP model approach (Burant, 2015).

This equation still contains some inherent errors. There is often experimental uncertainty associated with the measurement and calculation of Setschenow coefficients. An additional section in (Burant, 2015) involved the development of an additional equation for the prediction of CaCl2. This was motivated by the fact that CaCl2 is the second most abundant electrolyte after NaCl in most natural reservoir brines.

**Countercurrent Packed Tower Design**

Mass balance (MB) in countercurrent packed power:

Diagram

Description automatically generated

Figure 2: Mass balance in tower (Crittenden, 2012)

*MB (overall tower):*

*MB (transfer zone on the tower):*

Where:

Combination of terms in both Eq. 1 and Eq.2:

If the air used on the tower is clean (:

**Stripping Factor**

A parameter commonly used in the evaluation of packed towers is the stripping factor (S); S is defined as the ratio of the slope of the equilibrium line to the operating line slope. As shown in Fig. 14-14, the equilibrium line divided by the operating line yields the following expression for the S:

“*The optimal range for the stripping factor might be considered between 2 and 20 because high removal efficiency is not possible at S less than 1, and no additional improvements in removal occurs at values of S greater than about 20*” (Crittenden, 2012).

**Minimum air to water ratio**

The stripping factor can be related to the minimum air-to-water ratio when the treatment efficiency is very high can be approximated:

If assuming at least a 90% removal for a contaminant:

From (Crittenden, 2012): “*With respect to the selection of the optimum air-to-water ratio, it has been demonstrated that minimum tower volume and power requirements are achieved using approximately 3.5 times the minimum air-to-water ratio for contaminants with Henry’s law constants greater than 0.05 for high percentage removals, corresponding to a stripping factor of 3.5 (Hand et al., 1986).*”

**Packed-Tower Height**

The design equation for tower height can be derived using these assumptions:

1. steady-state conditions prevail in the tower.
2. air flow rate and water flow rate are constant through the column.
3. no chemical reactions occur.
4. plug flow conditions prevail for both the air and water.

*Liquid-phase MB (in the middle of the tower – interface between the water and air)*

*Assuming no chemical reaction occurs to generate organics inside the tower*

Mass transfer from the water to the media can be represented as follows:

Diagram

Description automatically generated

Figure 3: Mass balance in reaction interface

MB accounting for the reaction interface:

where:

The mass flux of solute A to an interface can be determined by:

Where:

The mass transfer coefficient depends on the diffusion coefficient and the mass transfer boundary layer thickness. The previous equation can be modified specifically for the two-film theory and accounting for the MB element:

Where:

Newly modified MB of the Air Stripping Tower:

Where:

Finalized formula with simplified approach accounting for the Stripping Factor (S) to determine the packed tower height (L):

Where:

In packed-tower aeration, the tower length is often defined as height of transfer unit (HTU) times the number of transfer units (NTU) or number of equilibrium stages:

Where the total length of the packed tower:

(Safety factor of 1.20 may be applied for entire column total height)

Typical packed tower heights usually do not exceed about 9 m (30 ft). Should the calculated tower length exceed 9 m, the air-to-water ratio could be increased by increasing the air flow rate to achieve the same treatment objective but with a smaller tower height (Edzwald, 2011).

**Determination of mass transfer coefficient KLa**

The determination of the overall liquid-phase mass transfer rate constant (KLa) is recommended to be determined experimentally. Yet, it can be predicted using the Onda correlation (Onda et al., 1968).

OTO Model (Onda et al., 1968):

OTO odel constraints (Crittenden, 2012):

OTO model nomenclature:

**Packed tower liquid and gas mass loading rate, pressure drop, and tower diameter**

The pressure drop correlations presented are valid for ΔP/L values between 50 and 1,200 Pa/m and it was presented (Edzwald, 2011). It’s important to note that in most cases the pressure drop constant is determined either using a generalized pressure drop curve for a random packed tower (Treybal, R. E. 1980. Mass Transfer Operations. Chemical Engineering Series, 3rd ed., McGraw-Hill, New York), the Eckert curve, or from the packing manufacturer provided pressure drop curves. For the purpose of this model, the following correlations were adapted from (Edzwald, 2011) to provide a prediction of the pressure drop constant to be utilized in the calculation of the gas mass loading rate equation:

Parameters to predict pressure drop are the following:

The parameter E is defined as follows:

The empirical parameter M is defined by the following relationship:

The gas mass loading rate is determined by:

The liquid mass loading rate is determined by:

The liquid and gas volumetric loading rate are determined by:

The packed tower cross sectional area is determined by:

The packed tower cross diameter is determined by:

Standard tower diameter sizes of 1.22 m (4 ft), 1.83 m (6 ft), 2.44 m (8 ft), 3.048 m (10 ft), 3.66 m (12 ft), and sometimes 4.27 m (14 ft) in diameter are usually the norm for most packed-tower equipment manufacturers (Crittenden, 2012).

Determine the volume of packed tower based on the area and length:

Determine the liquid superficial velocity:

**Determine the power requirements of the Air Stripping system**

The air flowrate is determined as follows:

The air mass flowrate is determined as follows:

Calculate the pressure drop through the demister, the packing support plate, duct work, and inlet and outlet:

Calculate the inlet pressure to the packed tower:

Calculate the blower brake power:

Calculate pump power requirements to move the water to the top of the tower:

Calculate total power requirements and specific energy:

**Determination of diffusion coefficients**

The Hayduk–Laudie correlation is used to determine the liquid-phase diffusion coefficient through the following empirical equation:

Where:

Molar volumes can be roughly estimated by the Tyn and Calus correlation method, with the inclusion of the VOC’s critical molar volume that can be obtained through reported chemical properties (Aniceto et al., 2021):

The diffusion coefficient of an organic compound in the gas phase can be calculated through the Wilke–Lee correlation (Wilke and Lee, 1955), which is a modification of the Hirschfelder–Bird–Spotz correlation (Hirschfelder et al., 1949).

Molecular separation at collision for component A (VOC), nm:

Energy of molecular attraction for component A, erg:

Where:

The diffusion coefficient of a substance when the stagnant gas B is air can be calculated by assuming that air behaves like a single substance with respect to molecular collisions. The required parameters for air are:

Determine the collision function:

Calculation of gas-phase diffusion coefficients with the Wilke–Lee correlation:

**Cost Package Development**

Capital cost relationships were adapted from (Dzombak et al., 2021; Dzombak et al., 1993) which are used on the air stripping design and costing (ASDC) software , and from additional sources in the literature (Smith, 2005):

Capital cost development based on the following design of air stripper in (Dzombak et al., 2021):

Diagram

Description automatically generated

Figure 4: Air stripper design of reference from (Dzombak et al., 2021)

Process equipment cost for aluminum reactor (Dzombak et al., 2021; Dzombak et al., 1993):

Where:

Access port (Dzombak et al., 2021; Dzombak et al., 1993):

The access ports are assumed to be of the same material as the column shell.

Where:

Inlet and outlet pipes (Liquid) (Dzombak et al., 2021; Dzombak et al., 1993):

Where:

Air inlet (Dzombak et al., 2021; Dzombak et al., 1993):

Tray rings cost (Dzombak et al., 2021; Dzombak et al., 1993):

In the assumed tower configuration, tray rings are used to support the liquid distributor and fiberglass-reinforced plastic (FRP) support plate (Dzombak et al., 2021).

Column internals cost (Dzombak et al., 2021; Dzombak et al., 1993):

The column internals include one plate-type liquid distributor, wall-wiper liquid redistributors (for every 5 to 6 feet), and one FRP packing support plate (Dzombak et al., 2021).

Packing material cost:

This is mostly dependent on the packing material manufacturer’s cost per volume of material. Typical materials can be:

* Plastic (PVC - most common)
* Ceramic
* Stainless steel

Costs adapted from (Towler & Sinnott, 2013) for different materials of the packing:

* PVC plastic = $5,500/m3
* Ceramic = $2,000/m3
* Stainless steel = $8,000/m3 (average)

Mist eliminator (Dzombak et al., 2021; Dzombak et al., 1993):

Water pump capital cost (Smith, 2005):

Air blower capital cost (Towler & Sinnott, 2013):

Administrative, laboratory, and building cost:

Sharma, J.R. (2010). Development Of a Preliminary Cost Estimation Method for Water Treatment Plants. [Link Here](https://rc.library.uta.edu/uta-ir/handle/10106/4924)

Operational costs:

**Appendix**

**Possible future incorporations into the model:**

Mass transfer correlation model #2: BS Model (Billet & Schultes, 1993; Billet & Schultes, 1999)

In addition to the Onda correlations, there are additional approaches to determine the KLa in air stripping and distillation design (Flagiello et al., 2021). A more thorough model to determine the KLa was developed by Billet and Shultes (Billet & Schultes, 1993; Billet & Schultes, 1999).

Model #2 nomenclature:

The height calculation of the BS model is as follows:

* For the overall HTU:

**Off-gas GAC treatment**

Air stripping is more economical than GAC for removal of VOCs if the off gas can be directly discharged without treatment (Ball and Edwards, 1992; Gross and TerMaath, 1985; Hand et al., 1986). The economic advantage of air stripping over GAC diminishes when off-gas treatment is required and other strategies should be investigated (Ball and Edwards, 1992). For the off-gas treatment development, the use of an approach provided in (Edzwald, 2011) is considered.

Assuming the relative humidity (RH) of the air stripper off-gas is 100%, it’s key to reduce the RH of the off-gas to at least 50% to treat the off-gas VOC through granular activated carbon (GAC). This is because high RH values cause a phenomenon called capillary condensation to take place where the water vapor can condense in the micropores of the GAC adsorbent and then compete with the VOCs for adsorption sites, and the VOC capacity of the adsorbent can be significantly reduced (Edzwald, 2011).

Since the assumption of RH of the off gas in the tower is 100%, then it can be assumed that the dew point temperature in the system will be equal to the gas temperature in K entering the tower:

Considering the previously established assumption, the temperature required to obtain a RH of 50% was calculated with the August-Roche-Magnus approximation presented in (Alduchov & Eskridge, 1996):

The Antoine-equation is used to determine the saturated vapor pressure of the chemical to be removed in the GAC:

Where the Antoine coefficients A, B, and C are obtained through the literature (Yaws & Satyro, 2015). In addition to the Antoine coefficients, the refractive indexes (**ƞ**) of each chemical are also obtained through the literature for the purpose of future calculations (Haynes, 2014). Table A1 presents both the Antoine coefficients and the refractive index of the default chemicals in the model dictionary.

Table A1: Additional chemical information for incorporation

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Chemical** | **Temp. Range, °C** | **A** | **B** | **C** | **Ƞ1** |
| Benzene | -9.60 to 103.04 | 6.81432 | 1090.4312 | 197.146 | 1.501 |
| Ethylbenzene | 24.75 to 163.83 | 7.15610 | 1559.5452 | 228.582 | 1.493 |
| Chlorobenzene | 20.41 to 159.63 | 7.17262 | 1571.7847 | 234.229 | 1.524 |
| Propylbenzene | 42.15 to 188.20 | 7.18167 | 1655.2071 | 225.615 | 1.489 |
| o-Dichlorobenzene | 57.59 to 211.57 | 6.96861 | 1595.0445 | 209.647 | 1.551 |
| m-Dichlorobenzene | 51.26 to 203.15 | 7.19056 | 1727.6279 | 227.815 | 1.545 |
| p-Dichlorobenzene | 50.42 to 204.54 | 7.26241 | 1805.1119 | 237.826 | 1.528 |
| Toluene | 5.65 to 136.67 | 7.13657 | 1457.2871 | 231.827 | 1.494 |
| Carbon Tetrachloride | -22.82 to 283.20 | 7.01101 | 1278.4541 | 232.888 | 1.460 |
| o-Dichloropropane | -5.76 to 122.24 | 7.17775 | 1448.2346 | 240.189 | 1.439 |
| m-Xylene | 27.82 to 166.65 | 7.18115 | 1573.0243 | 226.671 | 1.494 |
| o-Xylene | 32.17 to 172.28 | 7.14914 | 1566.5881 | 222.596 | 1.501 |
| p-Xylene | 13.26 to 165.91 | 7.15471 | 1553.9461 | 225.230 | 1.492 |
| Chloroform | -28.50 to 263.25 | 7.11289 | 1233.0732 | 230.213 | 1.446 |
| 1,1,1-Trichloroethane | -30.05 to 271.85 | 7.00849 | 1253.4670 | 229.624 | 1.431 |
| Methane | -196.85 to -82.59 | 6.84377 | 435.4534 | 271.361 | 1.270 |
| Carbon dioxide | -119.74 to -8.96 | 9.81367 | 1340.9768 | 271.883 | 1 |
| Ammonia | -77.74 to 132.50 | 7.58743 | 1013.7815 | 248.83 | 1 |

1. The refractive index of the VOC was obtained through CRC Handbook of Chemical Engineering – Physical Constants of Organic Compounds and online sources (only used when wanting to have an off-gas treatment approach).

The concentration of the removed chemical in the off gas is calculated as:

Calculate the gas-phase concentration entering the adsorber accounting for the required temperature increase:

The partial pressure of the VOC in the gas is calculated as:

The following is used to calculate the polarizability of the target chemical in the off gas:

Calculate the best possible GAC usage rate assuming no mass transfer resistance. Assume the adsorbent that will be used in the design will be one of the following (Edzwald, 2011):

A picture containing text, screenshot, font, line

Description automatically generated

Figure A1: Information of commercial gas-phase adsorbent for off-gas treatment

The adsorbed gas-phase concentration is in equilibrium with the gas-phase concentration is determined through the Dubinin-Raduskevich (D-R) equation which was shown to correlate the isotherms of several gas-phase VOCs (Crittenden, 2012; Edzwald, 2011) as follows:

The GAC usage rate is determined as follows:

The mass of the GAC is calculated as:

***Note****:*

* + Typical design parameters for gas-phase GAC fixed-bed adsorbers consist of empty bed contact times (EBCTs) from 1.5 to 5.0 seconds and air loading rates (us) from 0.25 to 0.50 m/s (0.82 to 1.64 ft/s) (Edzwald, 2011).
  + Bulk density in GAC media can range from 400 kg/m3 to 800 kg/m3.

The volume of gas treated in the GAC is determined by:

The GAC bed life is determined by the following:

The bed length based on velocity and EBCT is calculated as:

The bed area based on velocity and volumetric flow is calculated as follows:

The volume of the GAC contactor is:

Rate of new GAC mass required:

Heating energy required is calculated as:

***Note:***

* Specific heat capacity of air at constant pressure (Cp) = 1.01 kJ/kg K
  + <http://hvac-calculator.com/heating.php>
  + <https://www.engineeringtoolbox.com/heating-humid-air-d_693.html>

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