

A Physical Property Resource Tool for Water Treatment Unit Operations

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INTRODUCTION

- **SOFTWARE TO ESTIMATE PHYSICAL PROPERTIES (StEPP) IS A PHYSICAL PROPERTY RESOURCE TOOL FOR WATER TREATMENT UNIT OPERATIONS**
- **StEPP CAN PREDICT PHYSICAL AND CHEMICAL PROPERTIES OF OVER 1000 ORGANIC CONTAMINANTS FROM A DATABASE AND FROM VARIOUS PARAMETER ESTIMATION TECHNIQUES**
- **SEVERAL PROPERTIES IN StEPP ARE AVAILABLE OVER A WIDE RANGE OF TEMPERATURES**
- **StEPP IS DESIGNED FOR THE MICROSOFT WINDOWS INTERFACE WITH USER-FRIENDLINESS IN MIND, CONSISTING OF A VISUAL BASIC FRONT-END AND FORTRAN COMPUTATIONAL ROUTINES**

SAMPLE CLASSES OF COMPOUNDS AVAILABLE IN StEPP

ALKANES

CYCLOALKANES

ALKENES

CYCLOALKENES

ALKYNES

AMINES

AROMATICS

CARBOXYLIC ACIDS

ETHERS

ESTERS

THIOLS

ALCOHOLS

NITRILES

DIOXINS

PCBs

KETONES

ALDEHYDES

EPOXIDES

CHEMICAL PROPERTIES AVAILABLE FROM THE StEPP DATABASE:

- HENRY'S CONSTANT (*)
- MOLECULAR WEIGHT
- LIQUID DENSITY (*)
- REFRACTIVE INDEX
- OCTANOL WATER PARTITION COEFFICIENT
- VAPOR PRESSURE (*)
- NORMAL BOILING POINT
- MOLAR VOLUME (*)
- AQUEOUS SOLUBILITY

(*) - DENOTES TEMPERATURE-DEPENDENT PROPERTY

CHEMICAL PROPERTIES IN StEPP AVAILABLE FROM PARAMETER ESTIMATION TECHNIQUES:

- INFINITE DILUTION ACTIVITY COEFFICIENT (*)
- HENRY'S CONSTANT (*)
- LIQUID DENSITY (*)
- AQUEOUS SOLUBILITY (*)
- GAS DIFFUSIVITY (*)
- OCTANOL WATER PARTITION COEFFICIENT (*)
- MOLECULAR WEIGHT
- MOLAR VOLUME
- LIQUID DIFFUSIVITY (*)

(*) - DENOTES TEMPERATURE-DEPENDENT PROPERTY

PHYSICAL PROPERTIES OF AIR AND WATER IN StEPP AVAILABLE FROM CORRELATIONS

- WATER DENSITY (*)
- WATER VISCOSITY (*)
- WATER SURFACE TENSION (*)
- AIR DENSITY (*)
- AIR VISCOSITY (*)

(*) - DENOTES TEMPERATURE-DEPENDENT PROPERTY

MAIN StEPP WINDOW

StEPP - Software to Estimate Physical Properties

File Units About Help

Operating Conditions:

Pressure (Pa) 1.01325E+5

Temperature (C) 10

Available Contaminants:

79016 TRICHLOROETHYLENE

79016 TRICHLOROETHYLENE

79027 DICHLOROACETALDEHYDE

79094 PROPIONIC ACID

79107 ACRYLIC ACID

Find Find Next Occurrence

Select Current Contaminant

Selected Contaminants:

79016 TRICHLOROETHYLENE

79016 TRICHLOROETHYLENE

Unselect Current Contaminant

Properties of the Contaminant:

TRICHLOROETHYLENE

Vapor Pressure (Pa)	4.69E+03
Infinite Dilution Activity Coeff. (-)	8.12E+03
Henry's Constant (-)	0.230
Molecular Weight (kg/kmol)	131.39
Normal Boiling Point (NBP) (C)	87.0
Liquid Density (kg/m3)	1.56E+03
Molar Volume at Oper. T (m3/kmol)	0.0843
Molar Volume at NBP (m3/kmol)	0.102
Refractive Index (-)	1.4750
Aqueous Solubility (PPMw)	821
log Octanol Water Part. Coeff. (-)	2.38
Liquid Diffusivity (m2/s)	6.44E-10
Gas Diffusivity (m2/s)	7.89E-06

Properties of Air and Water:

Water Density (kg/m3)	999.75
Water Viscosity (kg/m/s)	1.31E-03
Water Surface Tension (N/m)	0.0742
Air Density (kg/m3)	1.25
Air Viscosity (kg/m/s)	1.72E-05

SAMPLE APPLICATION OF StEPP TO PACKED TOWER AERATION DESIGN

- **StEPP WILL BE USED TO SUPPLY AERATION SYSTEM ANALYSIS PROGRAM (ASAP) WITH THE PHYSICAL AND CHEMICAL PROPERTIES NEEDED TO PREDICT THE PERFORMANCE OF A PACKED TOWER**
- **THE ASAP PREDICTION WILL BE COMPARED WITH ACTUAL FIELD DATA FOR AN AIR STRIPPER OPERATED IN WAUSAU, WISCONSIN UNDER THE FOLLOWING CONDITIONS:**
 - **TEMPERATURE = 10 °C**
 - **PRESSURE = 101325 Pa**
 - **COMPOUNDS: TRICHLOROETHYLENE (TCE)
TETRACHLOROETHYLENE (PCE)
CIS-1,2-DICHLOROETHYLENE (DCE)**

ASAP - AERATION SYSTEM ANALYSIS PROGRAM

- **SIMULATE THE FOLLOWING POLLUTION PREVENTION TREATMENT TECHNOLOGIES: PACKED TOWER AERATION, BUBBLE AERATION, AND SURFACE AERATION**
- **ASAP ALLOWS FOR THE DESIGN AND RATING OF A PACKED TOWER AERATION SYSTEM, INCLUDING THE CAPABILITY TO OPTIMIZE A TOWER DESIGN FOR A GIVEN SET OF CONTAMINANTS**
- **ASAP ALLOWS FOR THE DESIGN AND RATING OF BUBBLE AND SURFACE AERATION SYSTEMS, INCLUDING THE ABILITY TO ACCOMMODATE TANKS IN SERIES**
- **LINKED TO A DATABASE OF RANDOM PACKING MATERIALS**
- **LINKED TO StEPP FOR THE RETRIEVAL OF CHEMICAL AND PHYSICAL PROPERTIES**

CHEMICAL PROPERTIES PROVIDED BY StEPP FOR ASAP SIMULATION

PROPERTY	DCE	TCE	PCE
Molecular Weight (kg/kmol)	96.94	131.39	165.84
Henry's Constant (-)	0.199	0.230	0.361
Normal Boiling Point (°C)	60.5	87.0	121.0
Molar Volume at NBP (m ³ /kmol)	0.0840	0.1020	0.1190
Liquid Diffusivity (m ² /sec)	7.20E-10	6.44E-10	5.86E-10
Gas Diffusivity (m ² /sec)	8.89E-06	7.89E-06	7.13E-06

AIR AND WATER PROPERTIES PROVIDED BY StEPP FOR ASAP SIMULATION

PROPERTY	VALUE
Water Density (kg/kmol)	999.75
Water Viscosity (kg/m/sec)	1.31E-03
Water Surface Tension (N/m)	0.0742
Air Density (kg/m ³)	1.25
Air Viscosity (kg/m/sec)	1.72E-05

COMPARISON OF FIELD DATA TO ASAP PREDICTION OF PACKED TOWER PERFORMANCE FOR WAUSAU STUDY

Compound	Date	Influent Conc. ($\mu\text{g/L}$)	Field Data		ASAP Prediction	
			Effluent Conc. ($\mu\text{g/L}$)	Percent Removal	Effluent Conc. ($\mu\text{g/L}$)	Percent Removal
DCE	8/8/84	70	2.9	95.9	2.1	97.0
	8/8/84	77	4.7	93.9	3.1	96.0
	10/1/84	90	2.3	97.4	2.4	97.3
TCE	8/8/84	66	1.0	98.5	2.2	96.7
	8/8/84	67	1.8	97.3	3.0	95.6
	10/1/84	72	1.1	98.4	2.2	96.9
PCE	8/8/84	69	1.0	98.6	2.2	96.8
	8/8/84	69	0.8	98.8	2.9	95.8
	10/1/84	52	0.8	98.5	1.6	97.0

SAMPLE APPLICATION OF StEPP TO THE DESIGN OF A GAS-PHASE GAC ADSORPTION UNIT

- **StEPP WILL BE USED TO SUPPLY ADSORPTION DESIGN SOFTWARE WITH THE PHYSICAL AND CHEMICAL PROPERTIES NEEDED TO PREDICT THE PERFORMANCE OF A GAC ADSORBER**
- **THE ADSORPTION DESIGN SOFTWARE PREDICTION WILL BE COMPARED WITH ACTUAL FIELD DATA FOR A GAS-PHASE ADSORBER DESIGNED TO TREAT THE OFF-GAS OF A PACKED TOWER OPERATED IN WAUSAU, WISCONSIN UNDER THE FOLLOWING CONDITIONS:**
 - **TEMPERATURE = 24 °C**
 - **PRESSURE = 101325 Pa**
 - **COMPOUNDS: TRICHLOROETHYLENE (TCE)
TETRACHLOROETHYLENE (PCE)**

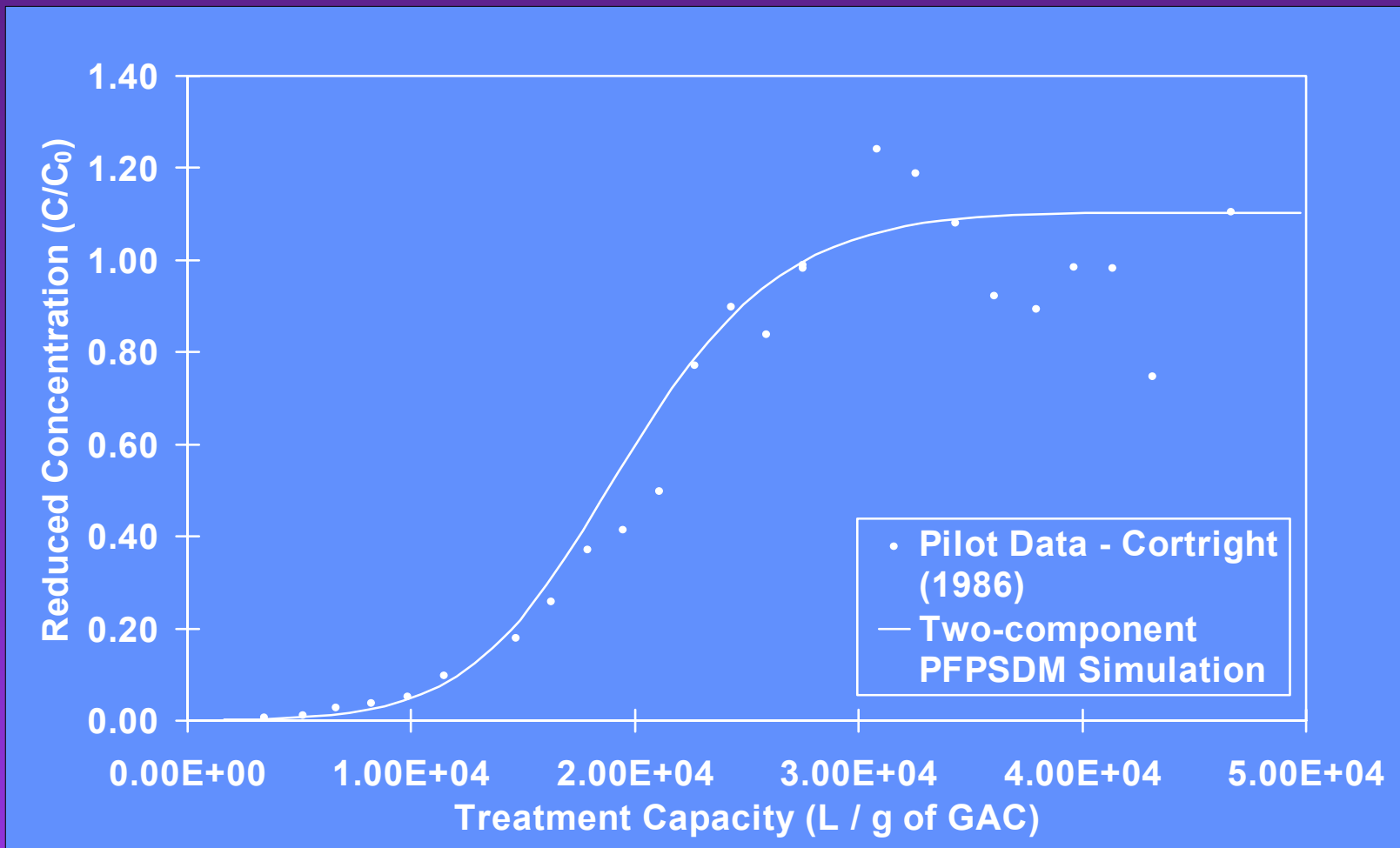
ADSORPTION DESIGN SOFTWARE

- **WINDOWS SOFTWARE WAS DEVELOPED TO HELP THE ENGINEER IN DESIGNING FIXED-BED ADSORBERS**
- **THE SOFTWARE IS DESIGNED TO APPLY THREE DIFFERENT FIXED-BED MODELS IN THE SIMULATION OF MULTICOMPONENT ADSORPTION OF CHEMICALS IN FIXED-BED ADSORBERS:**
 - **EQUILIBRIUM COLUMN MODEL (ECM)**
 - **CONSTANT PATTERN HOMOGENEOUS SURFACE DIFFUSION MODEL (CPHSDM)**
 - **PLUG-FLOW PORE AND SURFACE DIFFUSION MODEL (PFPSDM)**
- **SOFTWARE INCLUDES ADSORBENT AND ISOTHERM PARAMETER DATABASES TO PROVIDE THE USER WITH CHEMICAL AND ADSORBENT PROPERTIES**
- **LINKED TO StEPP FOR THE RETRIEVAL OF CHEMICAL AND PHYSICAL PROPERTIES**

CHEMICAL PROPERTIES PROVIDED BY StEPP FOR ADSORPTION DESIGN SOFTWARE PREDICTION

PROPERTY	TCE	PCE
Molecular Weight (kg/kmol)	131.39	165.84
Normal Boiling Point (°C)	87.0	121.0
Molar Volume at NBP (m ³ /kmol)	0.102	0.119
Liquid Density (kg/m ³)	1.53E+03	2.01E+03
Vapor Pressure (Pa)	9.38E+03	2.34E+03
Refractive Index (-)	1.4750	1.5055

COMPARISON OF FIELD DATA TO PFPSDM PREDICTION OF GAS-PHASE ADSORBER PERFORMANCE FOR TCE IN THE WAUSAU STUDY



FURTHER READING

Hokanson, D.R., T.N. Rogers, D.W. Hand, F. Gobin, M.D. Miller, J.C. Crittenden, and J.E. Finn, “A Physical Property Resource Tool for Water Treatment Unit Operations”, Proceedings of AWWA Annual Conference, pp. 411-422, Anaheim, CA, June 1995.

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DISCLAIMER

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