

Input Report

Workspace: Brenntag Portugal Estarreja_Dez21

Concrete, no bund

Pool substrate and bund

Brenntag Portugal Estarreja_Dez21\Pool substrates and bunds

Tab	Group	Field	Value	Units
Bund properties	Bund defined	Specify a bund	No	
	Dimensions	Bund height	0	m
		Bund area (internal)	0	m ²
		Bund diameter (internal)	0	m
	Whether the bund can overflow	Bund failure modeling		
		Bund area multiplier for catastrophic rupture	1,5	
Surface for pools	Type of surface for pools	Type of surface for pools	Concrete	
	User defined surface properties	Pool minimum thickness	5	mm
		Surface thermal diffusivity	9,48E-07	m ² /s
		Surface roughness factor	2,634	
		Surface thermal conductivity	0,00221	kJ/m.s.degK

Telheiro Zona de embalamento

Pool substrate and bund

Brenntag Portugal Estarreja_Dez21\Pool substrates and bunds

Tab	Group	Field	Value	Units
Bund properties	Bund defined	Specify a bund	Yes	
	Dimensions	Bund height	0,2	m
		Bund area (internal)	356,25	m ²
		Bund diameter (internal)	21,2977	m
	Whether the bund can overflow	Bund failure modeling	Bund cannot fail (liquid overfill not possible)	

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		Bund area multiplier for catastrophic rupture	1	
Surface for pools	Type of surface for pools	Type of surface for pools	Concrete	
	User defined surface properties	Pool minimum thickness	5	mm
		Surface thermal diffusivity	9,48E-07	m2/s
		Surface roughness factor	2,634	
		Surface thermal conductivity	0,00221	kJ/m.s.degK

Bacia 1 dos Misturadores

Pool substrate and bund

Brenntag Portugal Estarreja_Dez21\Pool substrates and bunds

Tab	Group	Field	Value	Units
Bund properties	Bund defined	Specify a bund	Yes	
	Dimensions	Bund height	0,4	m
		Bund area (internal)	13,7	m2
		Bund diameter (internal)	4,17653	m
	Whether the bund can overflow	Bund failure modeling	Bund cannot fail (liquid overflow not possible)	
		Bund area multiplier for catastrophic rupture	1	
Surface for pools	Type of surface for pools	Type of surface for pools	Concrete	
	User defined surface properties	Pool minimum thickness	5	mm
		Surface thermal diffusivity	9,48E-07	m2/s
		Surface roughness factor	2,634	
		Surface thermal conductivity	0,00221	kJ/m.s.degK

Bacia 2 dos Misturadores

Pool substrate and bund

Brenntag Portugal Estarreja_Dez21\Pool substrates and bunds

Tab	Group	Field	Value	Units
Bund properties	Bund defined	Specify a bund	Yes	
	Dimensions	Bund height	0,4	m
		Bund area (internal)	24	m2
		Bund diameter (internal)	5,52791	m
	Whether the bund can overflow	Bund failure modeling	Bund cannot fail (liquid overfill not possible)	
		Bund area multiplier for catastrophic rupture	1	
Surface for pools	Type of surface for pools	Type of surface for pools	Concrete	
	User defined surface properties	Pool minimum thickness	5	mm
		Surface thermal diffusivity	9,48E-07	m2/s
		Surface roughness factor	2,634	
		Surface thermal conductivity	0,00221	kJ/m.s.degK

Armázem de produto embalado

Pool substrate and bund

Brenntag Portugal Estarreja_Dez21\Pool substrates and bunds

Tab	Group	Field	Value	Units
Bund properties	Bund defined	Specify a bund	Yes	
	Dimensions	Bund height	0,2	m
		Bund area (internal)	500	m2
		Bund diameter (internal)	25,2313	m
	Whether the bund can overflow	Bund failure modeling	Bund cannot fail (liquid overfill not possible)	
		Bund area multiplier for catastrophic rupture	1	
Surface for pools	Type of surface for	Type of surface for	Concrete	

pools		pools		
	User defined surface properties	Pool minimum thickness	5	mm
		Surface thermal diffusivity	9,48E-07	m2/s
		Surface roughness factor	2,634	
		Surface thermal conductivity	0,00221	kJ/m.s.degK

Materials Report

Workspace: Brenntag Portugal Estarreja_Dez21

Material: ISOPROPANOL

Brenntag Portugal Estarreja_Dez21\Physical Properties
System\Materials\ISOPROPANOL

Property method template

PhastMC

General

Constants

Acentric factor	0,663	
Aerosol class number	11	
Critical pressure	47,65	bar
Critical temperature	235,15	degC
Flammable/Toxic flag	Flammable	
Melting point	-87,892	degC
Molecular weight	60,095	
Normal boiling point	82,15	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag	Soave	
Triple point pressure	1,69E-07	bar
Triple point temperature	-87,892	degC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	8,502E+07	1,474	-1,878	0,933	0	-87,892	235,15	1	Constant value above fraction Tc

Flammable

Constants

Combustion at	0,937291	
Combustion ct	0,044603	
Emissive power length scale	2,75	m

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Flash point	12	degC
Heat of combustion	1,834E+06	kJ/kmol
Immediate ignition category	Unknown	
Laminar burning velocity	0,52	m/s
Lower flammability limit	20000	ppm
Luminous/Smoky flame flag	General	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power	170	kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	127000	ppm

Toxic Constants

Dangerous dose 2		
Dangerous dose 3		
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes		
ERPG 1	0	ppm
ERPG 2	0	ppm
ERPG 3	0	ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	0	
Toxic property B	0	
Toxic property N	0	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal	100	0,20161	-0,00021	0	0	0	-87,892	151,85	1	Constant value

		529							above fraction Tc	
conductivity										
Liquid viscosity	101	-8,8918	2357,6	-0,91376	0	0	-87,89	82,15	1	Constant value above fraction Tc
Surface tension	106	0,044631	0,85552	0	0	0	-87,892	235,15	1	Constant value above fraction Tc
Vapour thermal conductivity	102	7,3907E-07	1,7419	0	0	0	82,15	726,85	1	None (use equation)
Vapour viscosity	102	1,2003E-06	0,494	479,78	0	0	-85,8	726,85	1	None (use equation)

Heat capacity

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	127	33260	796300	1001	101100	3286	-223,15	1226,85	1	None (use equation)
Liquid heat capacity	100	471710	-4172,1	14,745	-0,014402	0	-87,892	189,85	1	None (use equation)

Vapour pressure

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Vapour	101	110,7	-	-	5,538	2	-87,89	235,15	1	Vapour

Material: NITRIC ACID

Brenntag Portugal Estarreja_De21\Physical Properties System\Materials\NITRIC ACID

Property method template **PhastMC**

General Constants

Acentric factor	0,714406	
Aerosol class number	1	
Critical pressure	68,901	bar
Critical temperature	246,85	degC
Flammable/Toxic flag	Toxic	
Melting point	-41,6	degC
Molecular weight	63,0128	
Normal boiling point	83	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag	Soave	
Triple point pressure	0,000607682	bar
Triple point temperature	-41,6	degC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	7,06042E+07	0,692931	0	0	0	-41,6	86	1	Constant value above fraction Tc

Flammable Constants

Combustion at	1	
Combustion ct	1	
Emissive power length scale	0	m
Flash point		degC
Heat of combustion	13400	kJ/kmol
Immediate ignition category	Unknown	
Laminar burning velocity		m/s
Lower flammability limit	-9,95E+40	ppm

Luminous/Smoky flame flag	Non-flammable	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power	0	kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	-9,95E+40	ppm

Toxic Constants

Dangerous dose 2	1440	
Dangerous dose 3	5520	
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes	9,6	
ERPG 1	0,16	ppm
ERPG 2	24	ppm
ERPG 3	92	ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	-150,838	
Toxic property B	15,432	
Toxic property N	1	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal conductivity	100	0,12107	0,0005383	0	0	0	-40	160	1	Constant value above fraction Tc
Liquid viscosity	101	-28,886	1940	2,678	0	0	-6,10352E-06	94,75	1	Constant value above fraction Tc

Surface tension	100	0,08343	-	0	0	0	-	40	1	Constant value above fraction Tc
			0,0001455				6,10352E-06			
Vapour thermal conductivity	102	0,00063365	0,72057	645,24	0	83		726,85	1	None (use equation)
Vapour viscosity	102	2,2234E-07	0,72283	140,72	0	-41,6		726,85	1	None (use equation)

Heat capacity Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	107	33440	70500	1041	44700	473	-173,15	1226,85	1	None (use equation)
Liquid heat capacity	100	131250	-121,9	0,1704	0	0	-34,58	29,74	1	None (use equation)

Vapour pressure Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Vapour pressure	101	170,14	-10078	-22,769	2,73E-05	2	-41,6	102,95	1	Vapour Pressure Extrapolation

Density Coefficients

Name	Equation	A	B	C	D	Minimum	Maximum	Fraction	Supercritical
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	on					temperat ure [degC]	temperat ure [degC]	of critical temperat ure [fraction]	al extrapolat ion
Saturat ed liquid density	105	1,58 95	0,23 04	52 0	0,19 33	-41,6	100	1	Constant value above fraction Tc

Virial Coefficients

Name	Equatio n	A	B	C	D	E	Minimum temperatur e [degC]	Maximum temperatur e [degC]	Fraction of critical temperatur e [fraction]	Supercritical extrapolatio n
Second virial equation coefficien t	100	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Association Constants

Acid association flag	Not Modelled
Enthalpy interpolation range	0 delC

Coefficients

Name	Equatio n	A	B	C	D	E	Minimum temperatur e [degC]	Maximum temperatur e [degC]	Fraction of critical temperatur e [fraction]	Supercritical extrapolatio n
Dimer coefficient s	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Hexamer coefficient s	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Octamer coefficient s	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Trimer coefficient s	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Water Constants

Heat of solution	0	kJ/kg
Liquid water enthalpy coefficient A	0	
Liquid water enthalpy coefficient B	0	
Liquid water enthalpy coefficient C	0	
Liquid water enthalpy coefficient D	0	
Liquid water surface tension	0	N/m
Reaction with water model	None	
Solubility in water	0	
Water heat transfer coefficient	500	W/m ² .degK

Material: CARBON DIOXIDE

Brenntag Portugal Estarreja_De21\Physical Properties System\Materials\CARBON DIOXIDE

Property method template **PhastMC**

General Constants

Acentric factor	0,223621	
Aerosol class number	3	
Critical pressure	73,83	bar
Critical temperature	31,06	degC
Flammable/Toxic flag	Neither (Inert)	
Melting point	-56,57	degC
Molecular weight	44,0095	
Normal boiling point	-56,55	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag	Mathias	
Triple point pressure	5,18	bar
Triple point temperature	-56,57	degC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	2,173E+07	0,382	-0,4339	0,42213	0	-56,57	31,06	1	Constant value above fraction Tc

Flammable Constants

Combustion at	1	
Combustion ct	1	
Emissive power length scale	0	m
Flash point		degC
Heat of combustion		kJ/kmol
Immediate ignition category	Unknown	

Laminar burning velocity		m/s
Lower flammability limit	-9,95E+40	ppm
Luminous/Smoky flame flag	Non-flammable	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power	0	kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	-9,95E+40	ppm

Toxic Constants

Dangerous dose 2		
Dangerous dose 3		
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes		
ERPG 1	0	ppm
ERPG 2	0	ppm
ERPG 3	0	ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	-90,778	
Toxic property B	1,01	
Toxic property N	8	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal conductivity	100	0,4406	-0,0012175	0	0	0	-56,57	26,85	1	Constant value above fraction Tc
Liquid	101	18,77	-	-	-	1	-56,57	30	1	Constant

viscosity		5	402,92	4,68	6,917	0				value above fraction Tc
Surface tension	106	0,08414	1,284	0	0	0	-56,57	31,06	1	Constant value above fraction Tc
Vapour thermal conductivity	102	3,69	-0,3838	964	1,86E+06		-78,48	1226,85	1	None (use equation)
Vapour viscosity	102	2,148E-06	0,46	290	0		-78,48	1226,85	1	None (use equation)

Heat capacity

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	107	29370	34540	1428	26400	588	-223,15	4726,85	1	None (use equation)
Liquid heat capacity	100	-8,3043E+06	104370	-433,33	0,60052	0	-53,15	16,85	1	None (use equation)

Vapour pressure

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
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Vapour pressure	101	47,0169	-2839	-3,86388	2,81115E-16	6	-56,57	31,06	1	Vapour Pressure Extrapolation
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Density Coefficients

Name	Equation	A	B	C	D	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Saturated liquid density	105	2,768	0,26212	304,21	0,2908	-56,57	31,06	1	Constant value above fraction Tc

Virial Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Second virial equation coefficient	104	0,0478	-30,1	-2,173E+06	1,732E+18	-3,277E+20	-121,05	1247,85	1	None (use equation)

Association Constants

Acid association flag	Not Modelled
Enthalpy interpolation range	0 delC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature	Maximum temperature	Fraction of critical	Supercritical extrapolation
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Material: CARBON MONOXIDE

Brenntag Portugal Estarreja_De21\Physical Properties System\Materials\CARBON MONOXIDE

Property method template **PhastMC**

General Constants

Acentric factor	0,0481621	
Aerosol class number	2	
Critical pressure	34,99	bar
Critical temperature	-140,23	degC
Flammable/Toxic flag	Both	
Melting point	-205	degC
Molecular weight	28,0101	
Normal boiling point	-191,45	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag	Mathias	
Triple point pressure	0,154	bar
Triple point temperature	-205	degC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	8,585E+06	0,4921	-0,326	0,2231		0-205,02	-140,23	1	Constant value above fraction Tc

Flammable Constants

Combustion at	1,17361	
Combustion ct	0,295858	
Emissive power length scale	2,75	m
Flash point	-202,15	degC
Heat of combustion	283000	kJ/kmol
Immediate ignition category	Low	

Laminar burning velocity	0,45	m/s
Lower flammability limit	125000	ppm
Luminous/Smoky flame flag	General	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power	170	kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	742000	ppm

Toxic Constants

Dangerous dose 2	4980	
Dangerous dose 3	19800	
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes	4980	
ERPG 1	200	ppm
ERPG 2	350	ppm
ERPG 3	500	ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	-7,21	
Toxic property B	1	
Toxic property N	1	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal conductivity	100	0,2855	-0,001784	0	0	0	-205	-148,15	1	Constant value above fraction Tc
Liquid	101	-4,9735	97,67	-	0	0	-205	-141,78	1	Constant

viscosity				1,1088						value above fraction Tc
Surface tension	106	0,028898	1,16674	0	0	0	-205	-140,23	1	Constant value above fraction Tc
Vapour thermal conductivity	102	0,00059882	0,6863	57,13	501,92		-203,15	1226,85	1	None (use equation)
Vapour viscosity	102	1,1127E-06	0,5338	94,7	0		-205	976,85	1	None (use equation)

Heat capacity

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	107	29108	8773	3085,1	8455,3	1538,2	-213,15	1226,85	1	None (use equation)
Liquid heat capacity	114	65,429	28723	-847,39	1959,6	0	-205	-141,15	1	None (use equation)

Vapour pressure

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Vapour	101	45,6	-	-	7,567	2	-205	-140,23	1	Vapour

Dimer coefficient s	101	0 0 0 0 0	-273,15	-273,15	1	None (use equation)
Hexamer coefficient s	101	0 0 0 0 0	-273,15	-273,15	1	None (use equation)
Octamer coefficient s	101	0 0 0 0 0	-273,15	-273,15	1	None (use equation)
Trimer coefficient s	101	0 0 0 0 0	-273,15	-273,15	1	None (use equation)

Water Constants

Heat of solution	0	kJ/kg
Liquid water enthalpy coefficient A	0	
Liquid water enthalpy coefficient B	0	
Liquid water enthalpy coefficient C	0	
Liquid water enthalpy coefficient D	0	
Liquid water surface tension	0	N/m
Reaction with water model	None	
Solubility in water	4E-05	
Water heat transfer coefficient	500	W/m2.degK



Input Report

Workspace: Brenntag Portugal Estarreja_Dez21

Weather folder

Weather folder

Brenntag Portugal Estarreja_Dez21

Tab	Group	Field	Value	Units
General	Weather directions	Number of directions	8	
		Angular offset	0	deg
		Selection of directions to analyse	1; 1; 1; 1; 1; 1; 1; 1	

2.78/D

Weather

Brenntag Portugal Estarreja_Dez21\Weather folder

Tab	Group	Field	Value	Units
Weather	Weather conditions	Wind speed	2,78	m/s
		Pasquill stability	D neutral - little sun and high wind or overcast/windy night	
Atmospheric parameters	General atmospheric parameters	Atmospheric temperature	15,4	degC
		Relative humidity	0,8	fraction
		Solar radiation flux	0,5	kW/m2
	Mixing layer height vs. Pasquill stability	Mixing layer height for Pasquill stability A	1300	m
		Mixing layer height for Pasquill stability A/B	1080	m
		Mixing layer height for Pasquill stability B	920	m
		Mixing layer height for Pasquill stability B/C	880	m
		Mixing layer height for Pasquill stability C	840	m
		Mixing layer height for Pasquill stability C/D	820	m
		Mixing layer height for Pasquill stability D	800	m
		Mixing layer height for Pasquill stability E	400	m
		Mixing layer height for Pasquill stability F	100	m
		Mixing layer height for Pasquill stability G	100	m

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	Building data	Building exchange rate	4	/hr
		Tail time	1800	s
Substrate data	Surface temperature	Surface temperature for dispersion calculations	20,4	degC
		Surface temperature for pool calculations	20,4	degC