Input Report
Workspace: Brenntag Portugal Estarreja_Dez21
3600 s
Study
Brenntag Portugal Estarreja_Dez21

Tab	Group	Field	Value	Units
Context of calculations	Selection of context	Weathers to use for this study	Weather folder	
		Parameters to use for this study	3600s	
		Obstructions to use for this study		
Material	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Concrete, no bund	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
Dispersion	Distances of interest	Distances of interest		m

01 Rotura total de um GRG com ácido nítrico TEC, durante transporte por empilhador
Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	1340	kg
		Volume inventory	0,882737	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC

		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	

Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	0,882737	m3
		Tank vapour volume	0	m3
		Tank liquid volume	0,882737	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Concrete, no bund	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	

Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Geometry	Geometry	East	0	m
		North	0	m

Catastrophic rupture

Catastrophic rupture

Brenntag Portugal Estarreja_Dez21\3600 s\01 Rotura total de um GRG com ácido nítrico TEC, durante transporte por empilhador

Tab	Group	Field	Value	Units
Scenario	Release location	Elevation	0,1	m
		Tank head	0	m
	Fireball emissive power	Use vessel burst pressure	No	
		Vessel burst pressure - gauge		bar
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to model	Toxic only	

Discharge parameters	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Concrete, no bund	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

02 Fuga de 100 mm num GRG com ácido nítrico TEC, durante transporte por empilhador

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	1340	kg
		Volume inventory	0,882737	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	1	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m

		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	0,882737	m3
		Tank vapour volume	0	m3
		Tank liquid volume	0,882737	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	

		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Telheiro Zona de embalamento	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\02 Fuga de 100 mm num GRG com ácido nítrico TEC, durante transporte por empilhador

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	100	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	1	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to model	Toxic only	
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - continuous	Do not force correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	

Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Telheiro Zona de embalamento	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

03 Fuga de 10 mm num GRG com ácido nítrico TEC, durante transporte por empilhador

Atmospheric storage tank

Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	1340	kg
		Volume inventory	0,882737	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction

	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	1	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	

		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	0,882737	m3
		Tank vapour volume	0	m3
		Tank liquid volume	0,882737	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Telheiro Zona de embalamento	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	

		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\03 Fuga de 10 mm num GRG com ácido nítrico TEC, durante transporte por empilhador

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	10	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	1	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to	Toxic only	

		model		
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - continuous	Do not force correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Telheiro Zona de embalamento	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction

	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

04 Rotura catastrófica de um misturador com ácido nítrico

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	8040	kg
		Volume inventory	5,29642	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	

		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	5,29642	m3
		Tank vapour volume	0	m3
		Tank liquid volume	5,29642	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of		

		interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	

		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Geometry	Geometry	East	0	m
		North	0	m

Catastrophic rupture

Catastrophic rupture
Brenntag Portugal Estarreja_Dez21\3600 s\04 Rotura catastrófica de um misturador com ácido nítrico

Tab	Group	Field	Value	Units
Scenario	Release location	Elevation	0,1	m
		Tank head	0	m
	Fireball emissive power	Use vessel burst pressure	No	
		Vessel burst pressure - gauge		bar
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to model	Toxic only	
Discharge parameters	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	

		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

05 Fuga de 100 mm num misturador com ácido nítrico

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	8040	kg
		Volume inventory	5,29642	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component	PC modelling	

		modelling		
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	2,36	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar

	Inventory data for time-varying releases	Tank volume	5,29642	m3
		Tank vapour volume	0	m3
		Tank liquid volume	5,29642	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building	Buildings\Building type	

		type)		
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\05 Fuga de 100 mm num misturador com ácido nítrico

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	100	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	2,36	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to model	Toxic only	
	Phase	Phase to be released	Liquid	

Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - continuous	Do not force correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	

		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

06 Fuga de 10 mm num misturador com ácido nítrico

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	8040	kg
		Volume inventory	5,29642	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	2,36	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism -	Do not force correlation	

		continuous		
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	5,29642	m3
		Tank vapour volume	0	m3
		Tank liquid volume	5,29642	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined	No	

		averaging time		
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\06 Fuga de 10 mm num misturador com ácido nítrico

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	10	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	2,36	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to model	Toxic only	
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - continuous	Do not force correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m

	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

07 Rotura da linha de entrada no misturador com ácido nítrico

Pressure vessel

Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	8040	kg
		Volume inventory	5,29642	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Pressure/temperature	
		Temperature	20	degC

		Pressure (gauge)	8	bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head	0	

		losses		
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	5,29642	m3
		Tank vapour volume	0	m3
		Tank liquid volume	5,29642	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
	Safety system modelling for time-varying releases	Safety system modelling (isolation and blowdown)	No	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	

		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Geometry	Geometry	East	0	m
		North	0	m

Short pipe

Short pipe

Brenntag Portugal Estarreja_Dez21\3600 s\07 Rotura da linha de entrada no misturador com ácido nítrico

Tab	Group	Field	Value	Units
Scenario	Scenario	Scenario type	Line rupture	
	Pipe dimensions	Pipe internal diameter	76,2	mm
		Pipe length	12	m
	Hole	Orifice diameter		mm
	Release location	Elevation	0,1	m
		Tank head	0	m
	Flow control	Flow controller	None	
		Input option	Not applicable	
		Fixed flow rate		kg/s
		Pump head		m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to model	Toxic only	
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m

		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	

		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

08 Fuga na linha de entrada no misturador com ácido nítrico

Pressure vessel
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	NITRIC ACID	
		Specify volume inventory?	No	
		Mass inventory	8040	kg
		Volume inventory	5,29642	m3
		Material to track	NITRIC ACID	
	Phase	Specified condition	Pressure/temperature	
		Temperature	20	degC
		Pressure (gauge)	8	bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism -	Do not force correlation	

		continuous		
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	5,29642	m3
		Tank vapour volume	0	m3
		Tank liquid volume	5,29642	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
	Safety system modelling for time-varying releases	Safety system modelling (isolation and blowdown)	No	

Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time	0,05	fraction

		calculation		
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\08 Fuga na linha de entrada no misturador com ácido nítrico

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	7,62	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Toxic only	
		Material to track	NITRIC ACID	
		Type of risk effects to model	Toxic only	
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up	Droplet break-up	Do not force correlation	

	mechanism	mechanism - continuous		
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 2 dos Misturadores	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction

09 Rotura catastrófica de um misturador com álcool isopropílico

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	ISOPROPANOL	
		Specify volume inventory?	No	
		Mass inventory	3925	kg
		Volume inventory	4,98913	m3
		Material to track	ISOPROPANOL	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m

		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	4,98913	m3
		Tank vapour volume	0	m3
		Tank liquid volume	4,98913	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	

		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Explosion parameters	Explosion method (Consequence calculations only)	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	

		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Crosswind angle	0	deg
		Horizontal options	Use standard method	
		Correlation	Recommended	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s
Geometry	Geometry	East	0	m
		North	0	m

Catastrophic rupture

Catastrophic rupture
Brenntag Portugal Estarreja_Dez21\3600 s\09 Rotura catastrófica de um misturador com álcool isopropílico

Tab	Group	Field	Value	Units
Scenario	Release location	Elevation	0,1	m
		Tank head	0	m
	Fireball emissive power	Use vessel burst pressure	No	
		Vessel burst pressure - gauge		bar
Material	Material	Material characteristics	Flammable only	
		Material to track	ISOPROPANOL	
		Type of risk effects to model	Flammable only	
Discharge parameters	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
Explosion parameters	Explosion method	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	

		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s
	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	

		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s

10 Fuga de 100 mm num misturador com álcool isopropílico

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	ISOPROPANOL	
		Specify volume inventory?	No	
		Mass inventory	3925	kg
		Volume inventory	4,98913	m3
		Material to track	ISOPROPANOL	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	2,5	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	

		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	4,98913	m3
		Tank vapour volume	0	m3
		Tank liquid volume	4,98913	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass	1E+09	kg

		inventory		
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Explosion parameters	Explosion method (Consequence calculations only)	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion	Number of confined	0	

	sources	sources		
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Crosswind angle	0	deg
		Horizontal options	Use standard method	
		Correlation	Recommended	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	

	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s
Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	100	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	2,5	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Flammable only	
		Material to track	ISOPROPANOL	
		Type of risk effects to model	Flammable only	
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism -	Do not force correlation	

		continuous		
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
Explosion parameters	Explosion method	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3

		Volume fraction of confined source		fraction
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s
	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Correlation	Recommended	
		Horizontal options	Use standard method	
		Flame-shape adjustment if grounded	Yes	

	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s

11 Fuga de 10 mm num misturador com álcool isopropílico

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	ISOPROPANOL	
		Specify volume inventory?	No	
		Mass inventory	3925	kg
		Volume inventory	4,98913	m3
		Material to track	ISOPROPANOL	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	20	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m

	Release location	Elevation	0,1	m
		Tank head	2,5	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	4,98913	m3

		Tank vapour volume	0	m3
		Tank liquid volume	4,98913	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Explosion parameters	Explosion method (Consequence calculations only)	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass	Yes	

		modification factor		
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Crosswind angle	0	deg
		Horizontal options	Use standard method	
		Correlation	Recommended	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	

		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s
Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	10	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	2,5	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Flammable only	
		Material to track	ISOPROPANOL	
		Type of risk effects to model	Flammable only	
	Phase	Phase to be released	Liquid	

Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - continuous	Do not force correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
Explosion parameters	Explosion method	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	

		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s
	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	

		Jet fire maximum exposure duration	20	s
	Cone model data	Correlation	Recommended	
		Horizontal options	Use standard method	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s

12 Rotura da linha de entrada no misturador com álcool isopropílico

Pressure vessel

Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	ISOPROPANOL	
		Specify volume inventory?	No	
		Mass inventory	3925	kg
		Volume inventory	4,98913	m3
		Material to track	ISOPROPANOL	
	Phase	Specified condition	Pressure/temperature	
		Temperature	20	degC
		Pressure (gauge)	8	bar

		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	

		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	4,98913	m3
		Tank vapour volume	0	m3
		Tank liquid volume	4,98913	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
	Safety system modelling for time-varying releases	Safety system modelling (isolation and blowdown)	No	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and	Bacia 1 dos Misturadores	

		bunds		
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Explosion parameters	Explosion method (Consequence calculations only)	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	

		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s
	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Crosswind angle	0	deg
		Horizontal options	Use standard method	
		Correlation	Recommended	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2

		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s
Geometry	Geometry	East	0	m
		North	0	m

Short pipe

Short pipe

Brenntag Portugal Estarreja_Dez21\3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico

Tab	Group	Field	Value	Units
Scenario	Scenario	Scenario type	Line rupture	
	Pipe dimensions	Pipe internal diameter	76,2	mm
		Pipe length	12	m
	Hole	Orifice diameter		mm
	Release location	Elevation	0,1	m
		Tank head	0	m
	Flow control	Flow controller	None	
		Input option	Not applicable	
		Fixed flow rate		kg/s
		Pump head		m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material	Flammable only	

		characteristics		
		Material to track	ISOPROPANOL	
		Type of risk effects to model	Flammable only	
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for	ERPG [1 hr]	No	

	reports			
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
Explosion parameters	Explosion method	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction

	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s
	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Correlation	Recommended	
		Horizontal options	Use standard method	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	

		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s

13 Fuga na linha de entrada no misturador com álcool isopropílico

Pressure vessel

Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	ISOPROPANOL	
		Specify volume inventory?	No	
		Mass inventory	3925	kg
		Volume inventory	4,98913	m3
		Material to track	ISOPROPANOL	
	Phase	Specified condition	Pressure/temperature	
		Temperature	20	degC
		Pressure (gauge)	8	bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism -	Use flashing correlation	

		instantaneous		
		Droplet break-up mechanism - continuous	Do not force correlation	
Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	4,98913	m3
		Tank vapour volume	0	m3
		Tank liquid volume	4,98913	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg

	Safety system modelling for time-varying releases	Safety system modelling (isolation and blowdown)	No	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Explosion parameters	Explosion method (Consequence calculations only)	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification	Yes	

		factor		
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s
	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input	5	

		radiation levels		
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Crosswind angle	0	deg
		Horizontal options	Use standard method	
		Correlation	Recommended	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s
Geometry	Geometry	East	0	m
		North	0	m

Leak

Leak

Brenntag Portugal Estarreja_Dez21\3600 s\13 Fuga na linha de entrada no misturador com álcool isopropílico

Tab	Group	Field	Value	Units
Scenario	Hole	Orifice diameter	7,62	mm
		Use specified discharge coefficient?	No	
		Discharge coefficient		fraction
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Material	Material	Material characteristics	Flammable only	
		Material to track	ISOPROPANOL	
		Type of risk effects to model	Flammable only	
	Phase	Phase to be released	Liquid	
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - continuous	Do not force correlation	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building	Terrain and bund	Type of terrain for	Land	

and terrain	definition	dispersion		
		Type of pool substrate and bunds	Bacia 1 dos Misturadores	
Explosion parameters	Explosion method	Explosion method	Multi-Energy: User-defined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Multi-Energy	Multi-Energy: User-defined	Unconfined explosion strength	6	
		Unconfined explosion efficiency	100	%
	Confined explosion sources	Number of confined sources	0	
		Option for specifying size of confined sources	Use volumes	
		Strength of confined source		
		Volume of confined source		m3
		Volume fraction of confined source		fraction
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s

	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Correlation	Recommended	
		Horizontal options	Use standard method	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for	0,4	fraction

		general fires		
		Pool fire maximum exposure duration	20	s

14 Incêndio no armazém de produtos embalados

Atmospheric storage tank
Brenntag Portugal Estarreja_Dez21\3600 s

Tab	Group	Field	Value	Units
Material	Material	Material	CARBON MONOXIDE	
		Specify volume inventory?	No	
		Mass inventory	486	kg
		Volume inventory	1,64896	m3
		Material to track	CARBON MONOXIDE	
	Phase	Specified condition	Temperature and atmospheric pressure	
		Temperature	400	degC
		Pressure (gauge)		bar
		Fluid state	Liquid	
		Liquid mole fraction	1	fraction
	Modelling of mixtures	Multi or pseudo-component modelling	PC modelling	
Scenario	Pipe dimensions	Pipe length		m
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
Discharge parameters	Model settings	Atmospheric expansion method	DNV GL recommended	
		Phase change upstream of orifice?	Disallow liquid phase change only (metastable liquid)	
	Droplet break-up mechanism	Droplet break-up mechanism - instantaneous	Use flashing correlation	
		Droplet break-up mechanism - continuous	Do not force correlation	

Short pipe	Pipe characteristics	Pipe roughness	0,045	mm
	Frequencies	Frequency of bends in pipe	0	/m
		Frequency of couplings in pipe	0	/m
		Frequency of junctions in pipe	0	/m
	Frequencies of valves	Frequency of excess flow valves	0	/m
		Frequency of non-return valves	0	/m
		Frequency of shut-off valves	0	/m
	Velocity head losses	Excess flow valve velocity head losses	0	
		Non-return valve velocity head losses	0	
		Shut-off valve velocity head losses	0	
Time varying releases	Modelling of time-varying leaks and line ruptures	Vacuum relief valve	Operating	
		Vacuum relief valve set point	0	bar
	Inventory data for time-varying releases	Tank volume	1,64896	m3
		Tank vapour volume	0	m3
		Tank liquid volume	1,64896	m3
		Tank liquid level	0	m
		Maximum vapour release height		m
		Minimum mass inventory	0,1	kg
		Maximum mass inventory	1E+09	kg
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined		s

		averaging time		
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Armázem de produto embalado	
	Building definition	Release building		
		In-building release?	Outdoor	
		Building wake effect	Roof/lee	
		Wind or release angle from North	0	deg
		Handling of droplets	Trapped	
		Indoor mass modification factor	3	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06; 1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Explosion parameters	Explosion method (Consequence	Explosion method	Multi-Energy: Uniform confined	

	calculations only)			
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Crosswind angle	0	deg
		Horizontal options	Use standard method	
		Correlation	Recommended	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input	5	

		radiation levels		
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s
Geometry	Geometry	East	0	m
		North	0	m

User defined source

User defined source

Brenntag Portugal Estarreja_Dez21\3600 s\14 Incêndio no armazém de produtos embalados

Tab	Group	Field	Value	Units
Scenario	Release scenario	Release scenario	Leak	
		The number of release observers	2	
	Release observers	Release time	0; 3600	s
		Release phase	Vapour; Vapour	
		Mass flow	0,1; 0,1	kg/s
		Final velocity	0,9; 0,9	m/s
		Final temperature	20; 20	degC
		Liquid fraction	0; 0	fraction
		Droplet diameter		um
		Pool radius		m
		Pre-dilution air rate	1; 1	kg/s
		Downstream calculation status	No errors detected	
	Release location	Elevation	0,1	m
		Tank head	0	m
	Direction	Outdoor release direction	Horizontal	
		Outdoor release angle	0	deg
	Fireball emissive power	Use vessel burst pressure	No	

		Vessel burst pressure - gauge		bar
Material	Material	Material characteristics	Toxic and flammable	
		Material to track	CARBON MONOXIDE	
		Type of risk effects to model	Toxic and flammable	
Dispersion	Dispersion scope	Concentration of interest		ppm
		Averaging time for concentration of interest		
		Specify user-defined averaging time	No	
		User defined averaging time		s
	Distances of interest	Distances of interest		m
	Averaging time for reports	ERPG [1 hr]	No	
		IDLH [30 mins]	No	
		STEL [15 mins]	No	
Bund, building and terrain	Terrain and bund definition	Type of terrain for dispersion	Land	
		Type of pool substrate and bunds	Armázem de produto embalado	
Toxic parameters	Indoor toxic calculations	Specify the downwind building type	Unselected	
		Building type (downwind building type)	Buildings\Building type	
	Exposure time data	Set averaging time equal to exposure time	Use a fixed averaging time	
		Cut-off fraction of toxic load for exposure time calculation	0,05	fraction
		Cut-off concentration for exposure time calculations	0	fraction
	Toxic contours	Number of toxic levels	4	
		Dose levels	130000; 1,3E+06;	

			1,3E+07; 1,3E+08	
		Probit levels	2; 3; 4; 10	
		Lethality levels	0,001; 0,01; 0,1; 0,99	fraction
Explosion parameters	Explosion method	Explosion method	Multi-Energy: Uniform confined	
	Ignition	Supply late ignition location	No ignition location	
		Location of late ignition		m
	Vapour liquid method	Use explosion mass modification factor	Yes	
		Explosion mass modification factor	3	
Fireball	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Mass modification factor	3	
		Fireball maximum exposure duration	20	s
	Calculation method	Fireball model	Martinsen time varying	
		TNO model flame temperature	1726,85	degC
Jet fire	Jet fire method	Jet fire method	Cone model	
	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06;	

			2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Rate modification factor	3	
		Jet fire maximum exposure duration	20	s
	Cone model data	Correlation	Recommended	
		Horizontal options	Use standard method	
		Flame-shape adjustment if grounded	Yes	
	Surface emissive power	Calculation method for surface emissive power	Calculate SEP	
		Flame emissive power		kW/m2
		Emissivity fraction		fraction
Pool fire	Result types to calculate	Calculate probit	No	
		Calculate dose	No	
		Calculate lethality	No	
	Radiation levels	Number of input radiation levels	5	
		Intensity levels	37,5; 12,5; 7; 5; 3	kW/m2
		Probit levels	2,73; 3,72; 7,5	
		Dose levels	1,27E+06; 5,8E+06; 2,51E+07	
		Lethality levels	0,01; 0,1; 0,99	fraction
	Parameters	Radiative fraction for general fires	0,4	fraction
		Pool fire maximum exposure duration	20	s

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	m2
		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	m2/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	m2
		Bund diameter (internal)	21,2977	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

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 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

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

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**

conductivity			529							above fraction Tc
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		82,15	726,85	1	None (use equation)
Vapour viscosity	102	1,2003E-06	0,494	479,78	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
Vapou	101	110,7	-	-	5,538	2	-87,89	235,15	1	Vapour

r pressure		**17**	**9040**	**12,676**	**E-06**				**Pressure Extrapolation**

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**	**1,1799**	**0,2644**	**508,3**	**0,24653**	**-87,892**	**235,15**	**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**	**0,52914**	**-411,05**	**-3,258E+06**	**1,4421E+20**	**-8,859E+22**	**-19**	**1226,85**	**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 [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation

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

Water

Constants

Heat of solution	**20**	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	**1**	
Water heat transfer coefficient	**500**	W/m2.degK

Material: NITRIC ACID

Brenntag Portugal Estarreja_Dez21\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	-0,0001455	0	0	0	-6,10352E-06	40	1	Constant value above fraction Tc
Vapour thermal conductivity	102	0,000633 65	0,7205 7	645,24	0		83	726,85	1	None (use equation)
Vapour viscosity	102	2,2234E-07	0,7228 3	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	Equati	A	B	C	D	Minimum	Maximum	Fraction	Supercritic

	on					temperature [degC]	temperature [degC]	of critical temperature [fraction]	al extrapolation
Saturated liquid density	**105**	**1,5895**	**0,2304**	**520**	**0,1933**	**-41,6**	**100**	**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	**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	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Dimer coefficients	**101**	**0**	**0**	**0**	**0**	**0**	**-273,15**	**-273,15**	**1**	**None (use equation)**
Hexamer coefficients	**101**	**0**	**0**	**0**	**0**	**0**	**-273,15**	**-273,15**	**1**	**None (use equation)**
Octamer coefficients	**101**	**0**	**0**	**0**	**0**	**0**	**-273,15**	**-273,15**	**1**	**None (use equation)**
Trimer coefficients	**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/m2.degK

Material: CARBON DIOXIDE

Brenntag Portugal Estarreja_Dez21\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	4,6854	6,9171E-26	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

									]	
Vapour pressure	**101**	**47,0169**	**-2839**	**-3,86388**	**2,81115E-16**	**6**	**-56,57**	**31,06**	**1**	**Vapour Pressure Extrapolation**

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 temperatur	Maximum temperatur	Fraction of critical	Supercritical extrapolatio

							e [degC]	e [degC]	temperature [fraction]	n
Dimer coefficients	**101**	**0**	**0**	**0**	**0**	**0**	**-273,15**	**-273,15**	**1**	**None (use equation)**
Hexamer coefficients	**101**	**0**	**0**	**0**	**0**	**0**	**-273,15**	**-273,15**	**1**	**None (use equation)**
Octamer coefficients	**101**	**0**	**0**	**0**	**0**	**0**	**-273,15**	**-273,15**	**1**	**None (use equation)**
Trimer coefficients	**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	**0,00186**	
Water heat transfer coefficient	**500**	W/m2.degK

Material: CARBON MONOXIDE

Brenntag Portugal Estarreja_Dez21\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
Vapou	101	45,6	-	-	7,567	2	-205	-140,23	1	Vapour

r pressure		**98**	**1076,6**	**4,8814**	**3E-05**				**Pressure Extrapolation**

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**	**2,897**	**0,27532**	**132,92**	**0,2813**	**-205**	**-140,23**	**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**	**0,0506**	**-16,89**	**-70500**	**-1,39E+13**	**7,6E+14**	**-206,69**	**391,45**	**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 [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation

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

	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

Consequence Summary Report
Workspace: Brenntag Portugal Estarreja_Dez21
Study: 3600 s
Summary Basis

These tables will only report global values set in the parameters. Values that are modified in the study tree will not be reported.
The report is context sensitive, and filters up to the study level. You will need to generate multiple summary reports if you have multiple studies in your workspace.

Discharge Results (after atmospheric expansion)

Path	Scenario	Weather	Peak Flowrate [kg/s]	Temperature [degC]	Liquid mass fraction in material [fraction]	Droplet diameter [um]	Expanded diameter [m]	Velocity [m/s]	End time of release [s]
3600 s\01 Rotura total de um GRG com ácido nítrico TEC, durante transporte por empilhador	Catastrophic rupture	2.78/D		20	1	10000		0	
3600 s\02 Fuga de 100 mm num GRG com ácido nítrico TEC, durante transporte por empilhador	Leak	2.78/D	38,8551	19,9981	1	10000	0,0774597	5,43166	34,4871
3600 s\03 Fuga de 10 mm num GRG com ácido nítrico TEC, durante		2.78/D	0,388551	19,9981	1	10000	0,00774597	5,43166	3448,71

transporte por empilhador									
3600 s\04 Rotura catastrófica de um misturador com ácido nítrico	Catastrophic rupture	2.78/D		20	1	10000		0	
3600 s\05 Fuga de 100 mm num misturador com ácido nítrico	Leak	2.78/D	59,6914	19,9955	1	6015,3	0,0774597	8,3444	134,693
3600 s\06 Fuga de 10 mm num misturador com ácido nítrico		2.78/D	0,596914	19,9955	1	6015,3	0,00774597	8,3444	3600
3600 s\07 Rotura da linha de entrada no misturador com ácido nítrico	Short pipe	2.78/D	106,743	20,2434	1	1759,17	0,0762	15,4233	76,0997
3600 s\08 Fuga na linha de entrada no misturador com ácido nítrico	Leak	2.78/D	1,65388	19,8987	1	264,322	0,00590243	39,8136	3600
3600 s\09	Catastroph	2.78/D		20	1	10000		0	

Rotura catastrófica de um misturador com álcool isopropílico	ic rupture								
3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico	Leak	2.78/D	28,0602	19,9968	1	3835,05	0,0774597	7,56891	139,878
3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico		2.78/D	0,280602	19,9968	1	3835,05	0,00774597	7,56891	3600
3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico	Short pipe	2.78/D	76,8387	20,282	1	478,093	0,0762	21,4248	51,6413
3600 s\13 Fuga na linha de entrada no misturador com álcool isopropílico	Leak	2.78/D	1,04926	19,8677	1	92,5481	0,00590243	48,7356	3600

Dispersion Results

Input dispersion parameters

Core averaging time	18,75	s
Flammable averaging time	18,75	s
Toxic averaging time	600	s
Height of interest	0	m

Distance downwind to defined concentrations

The reported concentration of interest is defined at the scenario

Path	Scenario	Weather	Distance to UFL [m]	Distance to LFL [m]	Distance to LFL fraction [m]
3600 s\09 Rotura catastrófica de um misturador com álcool isopropílico	Catastrophic rupture	2.78/D	2,11707	2,13043	4,46456
3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico	Leak	2.78/D	1,58758	2,98219	8,45643
3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico		2.78/D	1,0663	1,23468	1,28275
3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico	Short pipe	2.78/D	2,29808	3,87415	8,11799
3600 s\13 Fuga na linha de entrada no misturador com álcool isopropílico	Leak	2.78/D	1,94399	2,47538	2,77637

Outdoor Toxic Results

Distance downwind to defined concentrations

The reported concentrations are defined in the respective material properties

Path	Scenario	Weather	Distance downwind to ERPG1 (3600 s) [m]	Distance downwind to ERPG2 (3600 s) [m]	Distance downwind to ERPG3 (3600 s) [m]	Distance downwind to STEL (900 s) [m]	Distance downwind to IDLH (1800 s) [m]
3600 s\01 Rotura total de um GRG com ácido nítrico TEC, durante transporte por empilhador	Catastrophic rupture	2.78/D	n/a	n/a	n/a	n/a	n/a
3600 s\02 Fuga de 100 mm num GRG com ácido nítrico TEC, durante transporte por empilhador	Leak	2.78/D	n/a	n/a	n/a	n/a	n/a
3600 s\03 Fuga de 10 mm num GRG com ácido nítrico TEC, durante transporte por empilhador		2.78/D	n/a	n/a	n/a	n/a	n/a
3600 s\04 Rotura catastrófica de um misturador com ácido nítrico	Catastrophic rupture	2.78/D	n/a	n/a	n/a	n/a	n/a
3600 s\05 Fuga de 100 mm	Leak	2.78/D	n/a	n/a	n/a	n/a	n/a

num misturador com ácido nítrico							
3600 s\06 Fuga de 10 mm num misturador com ácido nítrico		2.78/D	n/a	n/a	n/a	n/a	n/a
3600 s\07 Rotura da linha de entrada no misturador com ácido nítrico	Short pipe	2.78/D	n/a	n/a	n/a	n/a	n/a
3600 s\08 Fuga na linha de entrada no misturador com ácido nítrico	Leak	2.78/D	n/a	n/a	n/a	n/a	n/a
3600 s\14 Incêndio no armazém de produtos embalados	User defined source	2.78/D	n/a	n/a	n/a	n/a	n/a

Distance downwind to defined dangerous doses

The reported dangerous doses are defined in the respective material properties

Path	Scenario	Weather	Distance downwind to dangerous toxic load [m]	Distance downwind to dangerous dose 2 [m]	Distance downwind to dangerous dose 3 [m]
3600 s\01 Rotura total de um GRG com ácido nítrico TEC, durante transporte por empilhador	Catastrophic rupture	2.78/D	3814,74	193,103	78,4413
3600 s\02 Fuga de 100 mm num GRG com	Leak	2.78/D	3910,86	199,707	80,88

ácido nítrico TEC, durante transporte por empilhador					
3600 s\03 Fuga de 10 mm num GRG com ácido nítrico TEC, durante transporte por empilhador		2.78/D	2862,2	169,378	79,942
3600 s\04 Rotura catastrófica de um misturador com ácido nítrico	Catastrophic rupture	2.78/D	1695,19	99,8787	44,1354
3600 s\05 Fuga de 100 mm num misturador com ácido nítrico	Leak	2.78/D	1728,17	102,002	48,6887
3600 s\06 Fuga de 10 mm num misturador com ácido nítrico		2.78/D	669,286	83,7326	50,5302
3600 s\07 Rotura da linha de entrada no misturador com ácido nítrico	Short pipe	2.78/D	1814,63	112,853	60,9629
3600 s\08 Fuga na linha de entrada no misturador com ácido nítrico	Leak	2.78/D	1182,79	189,78	139,413
3600 s\14 Incêndio no armazém de produtos embalados	User defined source	2.78/D	113,857	113,857	58,4933

Exposure duration at defined dangerous doses

The reported dangerous doses are defined in the respective material properties

Path	Scenario	Weather	Exposure duration	Exposure duration	Exposure duration	Exposure duration	Exposure duration	Exposure duration

			for dangerous toxic load [s]	for dangerous dose 2 [s]	for dangerous dose 3 [s]	for dangerous dose 4 [s]	for dangerous dose 5 [s]	for dangerous dose 6 [s]
3600 s\01 Rotura total de um GRG com ácido nítrico TEC, durante transporte por empilhador	Catastrophic rupture	2.78/D	3106,21	3122,49	3136,5	n/a	n/a	n/a
3600 s\02 Fuga de 100 mm num GRG com ácido nítrico TEC, durante transporte por empilhador	Leak	2.78/D	3192,9	3198,11	3202,3	n/a	n/a	n/a
3600 s\03 Fuga de 10 mm num GRG com ácido nítrico TEC, durante transporte por empilhador		2.78/D	2746,47	2751,34	2769,39	n/a	n/a	n/a
3600 s\04 Rotura catastrófica de um misturador com ácido nítrico	Catastrophic rupture	2.78/D	3218,81	3216,57	3217,23	n/a	n/a	n/a

3600 s\05 Fuga de 100 mm num misturador com ácido nítrico	Leak	2.78/D	3282,62	3303,12	3310,58	n/a	n/a	n/a
3600 s\06 Fuga de 10 mm num misturador com ácido nítrico		2.78/D	3024,29	3048,75	3053,27	n/a	n/a	n/a
3600 s\07 Rotura da linha de entrada no misturador com ácido nítrico	Short pipe	2.78/D	3323,54	3318,65	3298,54	n/a	n/a	n/a
3600 s\08 Fuga na linha de entrada no misturador com ácido nítrico	Leak	2.78/D	3364,07	3286,68	3244,49	n/a	n/a	n/a
3600 s\14 Incêndio no armazém de produtos embalados	User defined source	2.78/D	3240	3240	3240	n/a	n/a	n/a

Jet Fire Results

Distance downwind to defined radiation levels

The reported radiations are defined in the parameters

Path	Scenario	Weather	Flame length [m]	Distance downwind to intensity level 1 (37,5 kW/m2) [m]	Distance downwind to intensity level 2 (12,5 kW/m2) [m]	Distance downwind to intensity level 3 (7 kW/m2) [m]	Distance downwind to intensity level 4 (5 kW/m2) [m]	Distance downwind to intensity level 5 (3 kW/m2) [m]
3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico	Leak	2.78/D	7,03604	n/a	7,86742	8,72181	9,41044	10,5879
3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico		2.78/D	1,52598	n/a	1,69377	1,69377	1,82094	2,05558
3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico	Short pipe	2.78/D	11,6702	12,9614	13,5838	15,6492	16,9656	19,2664
3600 s\13 Fuga na linha de entrada no misturador com álcool isopropílico	Leak	2.78/D	6,84975	7,66436	8,17454	9,33568	10,0966	11,4363

Early Pool Fire Results

Distance downwind to defined radiation levels

The reported radiations are defined in the parameters

Path	Scenario	Weather	Pool diameter [m]	Distance downwind to intensity level 1 (37,5 kW/m2) [m]	Distance downwind to intensity level 2 (12,5 kW/m2) [m]	Distance downwind to intensity level 3 (7 kW/m2) [m]	Distance downwind to intensity level 4 (5 kW/m2) [m]	Distance downwind to intensity level 5 (3 kW/m2) [m]
3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico	Leak	2.78/D	4,17665	2,58816	7,8006	9,78042	11,0979	13,5519
3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico		2.78/D	3,39299	2,50844	6,84344	8,52147	9,59389	11,6286
3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico	Short pipe	2.78/D	4,17659	2,58813	7,80051	9,7803	11,0977	13,5517
3600 s\13 Fuga na linha de entrada no misturador com álcool isopropílico	Leak	2.78/D	4,17663	2,58816	7,80058	9,78039	11,0978	13,5518

Late Pool Fire Results

Distance downwind to defined radiation levels

The reported radiations are defined in the parameters

Path	Scenario	Weather	Pool diameter [m]	Distance downwind to intensity level 1 (37,5 kW/m2) [m]	Distance downwind to intensity level 2 (12,5 kW/m2) [m]	Distance downwind to intensity level 3 (7 kW/m2) [m]	Distance downwind to intensity level 4 (5 kW/m2) [m]	Distance downwind to intensity level 5 (3 kW/m2) [m]
3600 s\09 Rotura catastrófica de um misturador com álcool isopropílico	Catastrophic rupture	2.78/D	4,17768	2,58878	7,80235	9,78257	11,1003	13,5549
3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico	Leak	2.78/D	4,17665	2,58816	7,8006	9,78042	11,0979	13,5519
3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico		2.78/D	4,17712	2,58845	7,8014	9,7814	11,099	13,5533
3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico	Short pipe	2.78/D	4,17659	2,58813	7,80051	9,7803	11,0977	13,5517
3600 s\13 Fuga na linha de entrada no	Leak	2.78/D	4,17663	2,58816	7,80058	9,78039	11,0978	13,5518

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Flash Fire Results

Distance downwind to defined concentrations

The reported LFL and LFL fraction are defined in the respective material property

Path	Scenario	Weather	Distance downwind to LFL [m]	Distance downwind to LFL Fraction [m]
3600 s\09 Rotura catastrófica de um misturador com álcool isopropílico	Catastrophic rupture	2.78/D	2,13043	4,46456
3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico	Leak	2.78/D	2,98219	8,45643
3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico		2.78/D	1,23468	1,28275
3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico	Short pipe	2.78/D	3,87415	8,11799
3600 s\13 Fuga na linha de entrada no misturador com álcool isopropílico	Leak	2.78/D	2,47538	2,77637

Maximum distance to LFL fraction at any height

Path	Scenario	Weather	Max flash fire distance [m]	Height of the max flash fire distance [m]	Time [s]
3600 s\09 Rotura catastrófica de um misturador com álcool isopropílico	Catastrophic rupture	2.78/D	4,25717	0	3,45237
3600 s\10 Fuga de 100 mm num misturador com álcool isopropílico	Leak	2.78/D	8,48486	0,025309	5,24077
3600 s\11 Fuga de 10 mm num misturador com álcool isopropílico		2.78/D	0,971685	0,0708938	3548,67

3600 s\12 Rotura da linha de entrada no misturador com álcool isopropílico	Short pipe	2.78/D	8,17699	0,0645196	51,3825
3600 s\13 Fuga na linha de entrada no misturador com álcool isopropílico	Leak	2.78/D	2,94505	0,0854089	3548,64