

Guideline on the
safety related requirements of the
ChemCar-Competition
Rev. 5

ChemCar 2017

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This guideline lists the documents and verifications that are required for the safety consideration of the submitted ChemCar concepts. Without these documents and verifications a qualified evaluation of the concepts is not possible and thus a security approval cannot be issued.

For clarification, an example of the documentation of the technical data of a ChemCar team in recent years is set at the end of this guideline. This example includes the calculations for estimating the developing reaction heat and the maximum pressure expected (see chapter 7-9). Please note that this example provides information only on the form and on the detail of the document but not on the content.

1. Pressure

- Operating pressure:
What is the pressure in normal operation of the ChemCar?
Here, it has to be specified if the pressure is indicated as absolute pressure ([bar]) or relative pressure ([bar_u])
- Maximum pressure expected:
How big can be the maximal achieved pressure at closed pressure vessels by the reaction?
Here, you have to consider the worst-case scenario.
- Pressure test/manufacturer certificate:
Attach the results of the pressure tests performed or a manufacturer certificate. When using a pressure system, a pressure test for the overall system might be necessary even if a manufacturer certificate is available. The requirements and the performance of the pressure test are specified in the ChemCar Safety Rules.
- Safety valve:
All the calculations for the design of the used safety valve (e.g. according to AD-Merkblatt A2) must be provided. Not only the results!
- Pressure gauge / pressure indicator
Ensure, that the ChemCar has a suitable pressure measurement / pressure indicator which has to be included in the process flowchart. It must be possible to read the internal pressure must at the ChemCars in any condition (e.g. in particular when the ChemCar breakdowns)

- In accordance with the ChemCar Safety Rules, you should pay attention that the pressure content product (pressure * volume) does not exceed 50 [bar*l] as far as possible. For the calculation, you have to use the maximum pressure expected. If the value exceeds 50 [bar*l], a consultation with the orgateam is recommended.

2. Temperature

- Maximum Temperature:
What is the maximal temperature expected during operation of the ChemCar?
All calculations and calculation basis must be indicated.
- Thermal hazard potential:
Do you reach flash points or ignition points of one or more substances?
Is there a risk, that thermal decomposition of one or more substances occur?
What decomposition products are formed?
What secondary reactions can take place?
How big is the resulting temperature in this case?
- Adiabatic temperature increase:
Is the reaction exothermic?
What reaction kinetics does the reaction have?
What temperature increase occurs under adiabatic conditions?
Here, the complete reaction of maximum quantities of the reactants must be taken as a basis.
- Hot surfaces:
What temperatures can be generated at accessible surfaces?
Is it possible that burns due to hot surfaces can occur (guideline: $T > 60^{\circ}\text{C}$)?
Is a contact protection necessary?
- Cold surfaces:
How cold do accessible surfaces get (by reactions or filling process)?
Is it possible to get injuries due to cold surfaces, e.g. frostbites or cold burns (guideline: $T < 0^{\circ}\text{C}$)
Is a contact protection necessary?

3. Emissions

- Exhaust emission:
Do exhaust gases release before, during or after operation
Which exhaust gases do release?
Which quantities are released in maximum (indicate calculations)?
What is the maximal released substance concentration in the surrounding area?
What are the limits for the released substance?
Is the ventilation sufficient?
- Noise emission:
What is the maximum noise level expected during operation?
Is it possible that injuries/impairments occur due to noise exposure (performer and viewers)?

4. Procedure

- Filling / dosing:
How is the reactor filled?
How are the educts dosed?
Is a wrong filling or wrong dosing possible?
What consequences can a wrong filling / dosing have?
- Leaks/ unintended release:
What dangers could be caused by a leak or accidental release?
What measures should be taken in case of a leak or an unintentional release?
What kind of protective equipment is necessary?
- Mechanical function:
How is the force transmitted?
What happens during a mechanical blockage? For example, the blocking of wheels?

5. Documentation

- Necessary documents:
 - A detailed functional description of the ChemCar
 - A photograph or drawing of ChemCar
 - A block flow diagram of the process
 - Safety Data Sheets of all existing substances (both used substances and produced)
 - H- and P-phrases (written form)
 - Summary of all used substances with quantities in a register of hazardous substances
 - P&ID of the ChemCar. Pay attention to completeness (piping, inscriptions etc.)
- Operating principle:
 - Description of the relevant system components (turbine, safety-bags etc.) and how they work
- Operating instructions:
 - Operating instructions according to TRGS 555 and GefStoffV § 14 for used reactants, products and potential auxiliaries. In the operating instructions the risks (explosive, oxidizing, toxic etc.), preventable conditions, transport, handling and disposal of the substance must be explained briefly. The minimum required personal protective equipment should be apparent from the operating instructions. An example of an operation instruction is shown in chapter 9.
 - A Safety Data Sheet is no operation instruction!!!
- Reaction Equation;
 - Indicate the complete reaction equation, including all side reactions and intermediates
- Calculations:
 - All calculation methods must be indicated (maximum temperature, maximum pressure, temperature increase etc.) and not only the results.
- Suitability of the material:
 - Are the used materials suitable?
 - Is a corrosion or embrittlement of material possible, caused by used or occurred substances?
 - Are the used materials suitable for the existing temperature ranges?

6. Risk assessment

The purpose of a risk assessment is the coverage of the intended use and any faults. The consequences of a disturbance are to refer to the specific application. A reference to the Safety Data Sheet (general application) is not enough!

In addition to those resulting hazards (e.g. explosion risk) caused from the used substances should be also substances considered, which can be caused by material properties (glass containers → splinter protection) or components (fast rotating components → cover).

Safety-Analysis Form:

Sequence of Steps	Potential Hazards	Procedure to Control Hazard	PPE or Equipment Required
Emergency shut-down			
	Hazard A (z. B. pressure increase)	Procedure A (z. B. stop educts supply , Opening of the safety valve)	PPE A, B, C (z. B. safety glasses, gloves and gowns)
Start-Up Procedure			
Run Time Procedure			
Shutdown Procedure			
Cleanup / Waste Disposal			

Example for a hazardous substances register:

Chemical Information Page

Fill in as much data below as available. **Be sure to list the units!** If data are not available, leave the field blank.
Material safety Datasheet (MSDS/SDS) for each named hazardous material is mandatory.

Chemical Quantities: List below the chemical names, concentrations, and total quantity of chemical required for the competition.

Chemical Name	Chemical State Solid, Liquid, Gas	Concentration Required	Total Quantity Required for Competition	Specific Personal Protective Equipment / Remarks

Chemical Properties and Hazards for ALL CHEMICALS, including reactants, solvents, intermediates and products.

Chemical Name	Physical State S, L, G	GHS Symbol(s)	H&P- Statements (No. only)		Incompatible Chemicals List chemicals present within the laboratory, and any others that may come in contact.	Flash Point Temp.
			Hazard Statements	Precautionary Statements		

7. Example: Calculation of the thermal risk potential

01	Parameter									
02	Route	20 m								
03	Time	30 s								
04	Geometry									
05	Wheel Diameter	0,2 m								
06	Piston Stroke	0,35 m								
07	Amount Of Rotations	31,83								
08	Cylinder Diameter	0,008 m								
09	Required Volume	0,00056 m ³								
10	Vehicle Data									
11	Weight	5 kg								
12	Additional Weight	0,3 kg								
13	Total Weight	6,5 kg								
14	Dynamic Calculation									
15	Kinetic Energy	1,44 J								
16	Speed	0,667 m/s								
17	Gravity Constant	9,81 m/s ²								
18	Coefficient Of Friction	0,6								
19	Friction Energy	765,18 J								
20	Efficiency	0,3								
21	Required Power	2555,41 W								
22	Required CO ₂ -Amount	1,01 mol								
23	Universal Gas Constant	8,314 J/mol/K								
24	Temperature	303,75 K								
25	Material Value									
26	Reaction	2 HCl + K ₂ CO ₃ -> 2 KCl + H ₂ O + CO ₂								
27	Educts	Mass	Mass Fraction	Molar Mass	Amount of	Stoichiometry	Gibbs Enthalpy	Enthalpy of For-	Volume	
		[g]		[g/mol]	Substance [mol]	Coefficient	[kJ/mol]	mation [kJ/mol]	[dm ³]	
28	Hydrochloric Acid	368,947	0,2	36,461	2024	-2	-93,8	-92,31		
29	Potassium Carbonate	289,637	0,5	138,21	1,048	-1	-1065,4	-1151		
30	Water	1765,424		18	98,079	1	-237,2	-285,83		
31	Products	Mass	Mass Fraction	Molar Mass	Amount of	Stoichiometry	Gibbs Enthalpy	Enthalpy of For-	Volume	
		[g]		[g/mol]	Substance [mol]	Coefficient	[kJ/mol]	mation [kJ/mol]	[dm ³]	
32	Carbon Dioxide	44533		44,01	1,012	1	-394,5	-393,5	22,67	
33	Potassium Chloride	150,875		74,551	2,024	2	-406,6	-436		
34	Water	18,214		18	1,012	1	-237,2	-285,8		
35	Molar Ratio	16,8947								
36	Reaction Value									
37	Reaction Heat	-872,450 kJ								
38	Gibbs Enthalpy	-191900 J/mol								
39	Excess Factor For Potassium Carbonate	1,036								
40	Reaction Conversion	1,000								
41	Experimentally Determined Volume	0,600 dm ³								
42	Adiabatic Temperature Increase									
43	Liquid Phase	3372,981 mol/m ³								
44	Concentration	-215680 J/mol								
45	Reaction Enthalpy	998,00 kg/m ³								
46	Heat Capacity	4184,00 J/kg/K								
47	Temperature Increase	174,22 K								
48	Generated Pressure									
49	"Free" Volume in Reactor	0,4211 dm ³								
50	Van-der-Waals Constant	0,3590 (Pam) ³ /mol ²								
51	a	0,0000427 m ³ /mol								
52	b	46,89 bar								
53	Pressure by Van-der-Waals	46,89 bar								

$$p \cdot V = R \cdot n \cdot T$$

$$\Delta T_{ad} = \frac{c_0^A \cdot (-\Delta_R H)}{\rho \cdot c_p}$$

$$p = \frac{n \cdot R \cdot T}{V - n \cdot b} - a \cdot \left(\frac{n}{V}\right)^2$$


To calculate the power, which is needed to absolve the required Route in addition of a given Weight, this calculation chart is used. The ideal gas law is used to charge the required amount of released gas to run a piston engine. The application quantity is given by the stoichiometry of the reaction. The correction is made by experimental Data. The heat capacity and the density is accepted as the value of Water, because all educts are in liquid Form or dissolved in this Phase.

8. Example for the design of a safety valve

Resource: AD2000-A2: SAFETY VALVE

01	Opening Pressure		1 bar _g		
02	Item Number			d ₀ = 18 mm, α = 0.54	
03	Reference				
04	Resource		A D2000-A2		
05	Nomination	Unit	Formula / Symbol	Value	Remark
06	Surroundings Data				
07	External Pressure	Pa	P_S	1,01E+05	
08	Internal Pressure	Pa	P_0	2,01E+05	1 bar _g
09	Temperature	K	T	293,15	
10	Passage Surface	m ²	A_0	0,0003	d = 18 mm
11	Effluent Number	-	α	0,54	
12	Thermodynamic Data				
13	Substance Notation			28,2 Vol.% NH ₃	mixture
14	Molar Mass	kg/mol	M	not necessary	
15	Compressibility	-	Z	0,889	
16	Isentropic Exponent	-	κ	1,4	
17	Results				
18	Maximal Mass Flow	kg/s	$\dot{m} = \alpha \cdot A_0 \cdot \psi \cdot \sqrt{2\rho_g P_0}$	2,26E-01	
19	Maximal Mass Flow	kg/h		8126,1807	
20	Maximal Volume Flow	Nm ³ /s	$\dot{V}_N = \frac{\dot{m}}{\rho_{gN}}$	1,38E-01	Standard Volume
21	Maximal Volume Flow	Nm ³ /h		497,014	
22	Flow Profile	-		critical	
23	Calculation Part				
24	Gas Density	kg/m ³	$\rho_g = \frac{P \cdot M}{R \cdot Z \cdot T}$	28,531	
25	Standard Gas Density	kg/m ³	$\rho_{gN} = \frac{101300[\text{Pa}] \cdot M}{R \cdot 273,15[\text{K}]}$	1,635	
26	Pressure Relation In/External	-	$\eta_0 = \frac{P_S}{P_0}$	0,503	
27	Critical Pressure Relation	-	$\eta_{crit} = \left(\frac{2}{\kappa+1}\right)^{\frac{\kappa}{\kappa-1}}$	0,528	
28	Pressure Relation	-	$\eta = \begin{cases} \eta_{crit} > \eta_0 \rightarrow \eta_{crit} \\ \eta_{crit} \leq \eta_0 \rightarrow \eta_0 \end{cases}$	0,528	
29	Effluent Function	-	$\psi = \sqrt{\left(\frac{\kappa}{\kappa-1} \cdot \left(\eta^{\frac{2}{\kappa}} \cdot \left(1 - \eta^{\frac{\kappa-1}{\kappa}}\right)\right)\right)}$	0,484	

9. Example for instruction manual according to TRGS 555

	Draft of the Instruction Manual	Date: Signature:
HAZARDOUS SUBSTANCE / OPERATIONS / WORKPLACE		
Hydrochlorid Acid, from 10 % to 25 %		
HAZARDS FOR HUMAN AND ENVIRONMENT		
	<p>Possibly corrosive against metal. (H290) Causes skin irritation. (H315) Causes heavy eye irritation. (H319) Possibly irritation of the air passages. (H335)</p> <p>- Inhalation, swallow or skin contact can cause health damages. Irritate the air passages, Eyes and Skin. Can cause damage to the gastrointestinal tract. Temporary caused cough, sickness and nasal smell disorder. Possibly damaged lungs, eyes, teethes, kidneys, gastrointestinal and laryngeal attacks.</p> <p>- Reacts with strong bases under emission of heat. Strong Reaction with sodium and potassium. Intensity and hazardousness of the reaction are influenced by the concentration of the acid. Reacts with amines, silicon oxide and water under emission of heat. Dangerous gases were generated by reaction with potassium manganite, sodium hypochlorite and concentrated sulphuric acid (e.g. chlorine, hydrogen chloride). Dangerous gases were generated by reaction with base metals (Hydrogen). Dangerous Gases were generated by reaction with carbonates (carbon dioxide). Emission of carbon dioxide: Danger of bursting in closed containers! Generating of harmful gases by reaction with nitrogen oxide (Dichloride dimethyl ether).</p> <p>- WGK: 1 (low hazardous of water)</p>	
SAFEGUARDING AND BEHAVIOURAL RULE		
	<p>- Activate the aspiration and work in its support by emission of damping or haze. Do not leave bundles and barrels open! Avoid splashing and trail by filling and decanting. Hold reactive substances off and add them only safely. Add the water first and afterwards the acid by dissolving and diluting! Control Temperature! Use acid-resistant equipment! Use utensils which protect the skin.</p> <p>- Do not eat, drink, smoke or sniff. Avoid inhalation of damping and aerosols! Avoid contact with eyes and skin! Clean hands and other contaminate body parts before taking a pause and the end of work. Use skin care products after the work! Rapidly remove product residues from the skin, clean and towel the concerned skin. Do not wear hand or arm decoration. Separately store street and work clothes! Rapidly shift contaminate and soaked work clothes. Use separate cleaning rags and wipes for skin and machines.</p> <p>- Follow the storage conditions! - Mind employment conditions!</p> <p>Supplies at workplace:</p> <p>- Eye protection: Using frame glasses with side protection by monitoring activity! Basket-shaped glasses by risk of splashing! - Hand protection: Gloves made of a suitable Material in response of the activity. It is advisable to wear cotton-made undergloves under the protection gloves! Considering the gestation periods of the protection gloves! Using special skin protectant by wearing of the longer term! - Breath protection: Combination filter E-P2 (yellow/white) or BE-P2 (grey/yellow/white) - Body protection: Wearing of an synthetic apron by diluting or bottling!</p>	
BEHAVIOUR BY EMERGENCY		FIRE SERVICE 112
<p>- Vacating and cordoning off the danger zone; inform the supervisor. - Wearing eye, hand and by great amounts breath protection to remove leaked or splashed substances. Soaking up with acid binding substances, disposal and residues are washed away with water! - Dangerous vapors are formed by fire (e.g. hydrogen chloride)! Leaking vapors deposit with spray water; then fast cleaning. Product is not flammable. Danger of Explosion by heating! - Preventing intrusion in ground, water and canalization! - Respecting alarm, escape and emergency routes. Alert fire service!</p> <p>Competent Doctor: Accident Telephone:</p>		
FIRST AID		EMERGENCY CALL 110
	<p>By every first aid measure: Mind self-protection, arrange medical treatment. Life saving emergency measures have to performed situational like recovery position, cardiopulmonary resuscitation or shock control. Sterile covering wounds. Resting the body and protecting for heat loss.</p> <p>After eye contact: Immediately, the eye has to rinsed for minimum 10 minutes by opened eyelid and protected uninvolved eye.</p> <p>After skin contact: Taking off contaminated clothes, even underwear and shoes, wearing personal protection utilities. Rinsing the skin with much water.</p> <p>After Inhalation: Take the injured out of the dangerous zone. Fresh air supply by breathing of fresh air or ventilation. Using resuscitation device (self protection). Immediately, even by missing signs of diseases, using a steroid (Dosier aerosol) for inhaling (in spray form). Dosage, kind of use and further treatment according to medical prescription.</p> <p>After swallow: Directly flush out the mouth. Drink water in small gulps.</p> <p>First aiders:</p>	
PROPER DISPOSAL		

10. References

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2. <http://www.dguv.de/ifa/GESTIS/GESTIS-Stoffdatenbank/index.jsp> GESTIS-Stoffdatenbank: Gefahrstoffinformationssystem der Deutschen Gesetzlichen Unfallversicherung
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4. <http://www.baua.de/de/Themen-von-A-Z/Gefahrstoffe/TRGS/TRGS-555.html> TRGS 555 "Betriebsanweisung und Information der Beschäftigten" (PDF-Datei, 98 KB)
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