PERIÓDICO TCHÊ QUÍMICA
NOTA

REFLETINDO SOBRE O DESCARRILAMENTO EM OHIO, EUA.

REFLECTING ON THE DERAILMENT IN OHIO, USA.

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RESUMO

Introdução: Em 3 de fevereiro de 2023, ocorreu um descarrilamento de trem em Ohio, causando um grande vazamento químico. O trem transportava vários compostos químicos que são matérias-primas para a indústria química, e devido ao descarrilamento, alguns vagões pegaram fogo e outros estavam em perigo de explosão devido ao superaquecimento. **Objetivos:** Esta nota tem como objetivo refletir sobre o estudo dos produtos químicos presentes no descarrilamento e se poderia haver um resultado diferente. **Métodos:** Foi feita uma breve pesquisa na internet, buscando informações sobre o descarrilamento e os principais produtos químicos que o trem estava transportando. As informações sobre os produtos químicos foram selecionadas a partir da Ficha de Dados de Segurança do Material (FDS) de fornecedores regulares dos produtos. **Resultados:** As informações coletadas sobre o descarrilamento eram pouco claras sobre as razões do fato, e a literatura sobre os produtos químicos apontava que a situação poderia piorar ou ser ainda pior do que já era. **Discussão:** No momento do estudo, não havia informações conclusivas disponíveis sobre as razões do descarrilamento. O vazamento de um agente carcinogênico tornou o cenário do descarrilamento mais difícil de operar. A combustão do cloreto de vinila pode criar gás fosgênio (aparentemente aconteceu) e aumentar o horror que se desdobrou no local do descarrilamento. **Conclusões:** A população local estava sofrendo na época e aguardando um apoio adequado. A equipe da locomotiva seguiu as regulamentações da empresa, e o pessoal que trabalhava no solo seguiu as ordens. Portanto, essas não parecem ser as razões para o descarrilamento.

Palavras-chave: *Descarrilamento em Ohio, acidente químico, fosgênio, compostos cancerígenos*

ABSTRACT

Background: On February 3, 2023, a train derailment happened in Ohio, causing a massive chemical spill. The train was transporting several chemical compounds that are raw materials for the chemical industry, and due to the derailment, some wagons caught fire, and others were in danger of explosion due to overheating. **Aims:** This note aims to reflect on the study of the chemicals present in the derailment and whether it could be a different outcome. **Methods:** A simple survey was done on the internet, looking for information about the derailment and the main chemicals the train was carrying. The information about the chemicals was selected from the Material Safety Data Sheet (MSDS) from regular suppliers of the products. **Results:** The information collected regarding the derailment was unclear about the reasons for the fact, and the literature regarding the chemicals pointed out that the situation could get worse or worse than it already was. **Discussion:** at the time of the study, no conclusive information was available regarding the reasons for the derailment. The spill of a carcinogenic agent turned the derailment scenario more difficult to operate. The combustion of vinyl chloride can create phosgene gas (apparently did it) and increase the horror show that unfolded at the derailment site. **Conclusions:** The local population was suffering at the time and waiting for real proper support. The locomotive crew followed the company regulations, and the personnel working on the ground followed orders. Therefore, those do not appear to be the reasons for the derailment.

Keywords: *Ohio derailment, chemical accident, phosgene, carcinogenic compounds.*

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1. INTRODUCTION

On February 3, 2023, a train derailed in East Palestine, Ohio, causing a massive fire. The reasons for such a catastrophic derailment are not apparent until now. Under such extraordinary conditions, it is not fair to consider evaluating the decisions taken by the ground personnel that was working under extreme danger, including the possibility of an unprecedented explosion.

Even so, the question of how the accident happened must be explained. Some hypotheses for the case may include mechanical failure, poor maintenance of the rails, insufficient workers, excessive number of cars in the same composition, sabotage, political motivation, and the use of substandard products to cut costs, among other possibilities. Despite the reasons for the derailment, what can be learned to prevent it from happening again?

Journalists from the USA have listed some of the chemicals spilled or burned in the derailment, which can be summarized in Table 1 (Bella Isaacs-Thomas, 2023; Brian McGill et al., 2023; Avery Koop, 2023).

An overview of the Material Safety Datasheet (MSDS) of those chemicals can provide the following information:

- **Vinyl chloride** (*Vinyl chloride, 1999*):

The hazards of combustion products, vinyl chloride forms highly toxic combustion products such as hydrogen chloride, phosgene, and carbon monoxide. It is also incompatible with oxidizers.

The inhalation of vinyl chloride in high concentrations causes dizziness, anesthesia, and lung irritation, and skin contact may cause frostbite.

- **Isobutylene** (Gas Innovations., 2015):

Flammable properties and hazards. The combustion of Isobutylene at high temperatures and proper fire conditions can form carbon monoxide (CO) and carbon dioxide (CO_2).

As a potential health effect, isobutylene is a simple asphyxiant. A simple asphyxiant is a gas or vapor that can displace oxygen in the air and lead to oxygen deprivation if it is in high enough concentrations. Simple asphyxiants do not have any toxic effects, but they can be dangerous in confined or poorly ventilated spaces where they can accumulate and displace the breathable air. The inhalation of high concentrations may cause rapid respiration, dizziness, fatigue, and nausea. Massive exposure may cause unconsciousness and death. Contact with the liquid phase or with the cold gas escaping from a cylinder may cause frostbite.

- **Butyl acrylate** (Safety Data Sheet - Fisher SCI., 2015):

The hazardous decomposition products of Butyl acrylate include carbon monoxide (CO) and carbon dioxide (CO_2). The materials that are incompatible with butyl acrylate include strong oxidizing agents, strong acids, strong bases, and peroxides.

The overexposure symptoms may include headaches, dizziness, tiredness, nausea, and vomiting. The symptoms of allergic reactions may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain, or flushing.

- **Benzene** (Sigma-Aldrich, 2023):

Benzene is a highly flammable liquid, and warming conditions must be avoided. The vapors of benzene may form explosive mixtures with air. There is a possibility of hazardous reactions in the presence of light metals, where light metals are metals with relatively low density, typically less than 5 g/cm³, such as aluminum, magnesium, titanium, and beryllium. It promotes exothermic reactions with halogens and halogenated hydrocarbons. During the reaction, there is a risk of explosion with halogen-halogen compounds, nitric acid, boranes, ozone, peroxy compounds, perchlorates, permanganic acid, perchloryl fluoride, strong oxidizing agents, chlorine, fluorides, uranium hexafluoride, and liquid oxygen.

Skin contact irritates. It causes damage to organs through prolonged or repeated exposure. It may cause genetic defects and may cause cancer.

- **DIETHYLENE GLYCOL** (Fisher SCI., 2021):

Diethylene glycol is incompatible with strong oxidizing agents, strong acids, and metals. The hazardous decomposition products are carbon monoxide (CO) and carbon dioxide (CO_2).

The symptoms of overexposure to diethylene glycol may include headache, dizziness,

tiredness, nausea, and vomiting.

- **Ethylene glycol monobutyl ether** (Fisher SCI², 2021):

The hazardous products of ethylene glycol monobutyl ether combustion are carbon monoxide (CO), carbon dioxide (CO_2), and peroxides.

Note that this product is air and light-sensitive. Avoid direct sunlight, exposure to air or moisture over prolonged periods, and heating in the air. It should be kept away from open flames, hot surfaces, and ignition sources. It is incompatible with strong oxidizing agents, bases, metals, and aluminum.

The symptoms of overexposure may include headache, dizziness, tiredness, nausea, and vomiting.

- **2-Ethylhexyl acrylate** (BASF, 2015):

2-Ethylhexyl acrylate forms explosive gas/air mixtures. The ignitable air mixtures can form when the product is heated above the flash point and when it is sprayed or atomized. Under confined conditions, there is the risk of explosion and fire hazards. Spontaneous and violent self-polymerization is risky if the inhibitor is lost, the product is exposed to excessive heat, or in the presence of UV radiation. The polymerization produces gases that may burst closed or confined containers. The reactions may cause ignition.

The materials incompatible with 2-Ethylhexyl acrylate include radical formers, free radical initiators, peroxides, mercaptans, nitro-compounds, perborates, azides, ether, ketones, aldehydes, amines, nitrates, nitrites, oxidizing agents, reducing agents, strong bases, acid anhydrides, acid chlorides, concentrated mineral acids, metal salts.

Radical formation can cause exothermic polymerization. It reacts with peroxides and other radical components. There is a risk of spontaneous polymerization in the presence of starters for radical chain reactions (e.g., peroxides). It polymerizes explosively in contact with Strong oxidizing agents. There is the risk of spontaneous polymerization in the presence of oxidizing agents.

It causes skin irritation, may cause allergic skin reactions, may cause respiratory irritation. It is harmful and toxic to aquatic life with long-lasting effects.

- **PROPYLENE GLYCOL** (Fisher SCI³, 2021):

Under intense heating, propylene glycol forms explosive mixtures with air. Hazardous reactions with oxidizing agents, acid anhydrides, and acid chlorides are a possibility.

The product is not listed as a carcinogenic agent.

2. DEVELOPMENT

All this information is interesting, but what role can this data play during the derailment? So, let us create a short list of problems to better visualize the situation:

1) There is a great spill of class 1A carcinogenic at the derailment site. The presence of chemicals that may form explosive mixtures with air. At least one chemical is an asphyxiant, and combustion reactions that are creating other chemicals that may be toxic or react with the original chemical compounds present in the area. The situation is very dynamic and could evolve in unpredictable forms.

2) It tends to have a negative psychological effect on the ground personnel. From what could be understood from the news on the media, the first responders possibly found an uncontrollable situation in the derailment.

3) At the derailment site, there were the presence of several chemical compounds that should not be heated, and they were catching fire (e.g., vinyl chloride, benzene, propylene glycol). Additionally, those chemicals were present in huge volumes. Some of the substances may create explosive mixtures with the air, and it may lead to a big explosion;

4) Some of the products may react in the presence of daylight, and they may be leaking in under pressure in the form of a spray. E.g., ethylene glycol monobutyl ether, when exposed to sunlight or ultraviolet light, can undergo photooxidation, which can cause the molecule to break down into smaller and potentially harmful compounds such as formaldehyde and formic acid. It is impossible to be 100% sure if this type of reaction could

have occurred in the derailment, but the conditions could not also be 100% eliminated.

5) Some chemical compounds (Ethylene glycol monobutyl ether, and Diethylene glycol) may react with metals, such as Aluminum and Iron. Usually, trains and railways are manufactured using those metals. The reaction of those compounds with these metals may lead to aluminum corroding and weakening, reducing its strength and structural integrity. And the iron can undergo a corrosion and rusting process. A weakened structure may not hold the chemicals properly, leading to other possible issues, such as an abrupt increase in leakage.

6) At the derailment site, some unwanted reactions and cross-actions were occurring or waiting to occur. Let us see some cases:

   a. Combustion of the vinyl chloride, as in Equation 1:

$2C_2H_3Cl + 7O_2 \rightarrow 4CO_2 + \mathbf{2HCl}$ (Eq. 1)

Note: HCl (strong acid**)**

   b. Combustion of the vinyl chloride in low oxygen conditions may lead to incomplete combustion, resulting in the formation of partially oxidized compounds such as carbon monoxide (CO). The carbon monoxide can potentially react with the original material, forming other compounds. For example, carbon monoxide can react with vinyl chloride to form phosgene gas ($COCl_2$), a combat gas, as in Equation 2.

$C_2H_3Cl + CO \rightarrow \mathbf{COCl_2} + H_2$ (Eq. 2)

Note: $COCl_2$ (chlorinated compound / halogenated hydrocarbon**)**

   c. A simplified equation of the combustion reaction of Ethylene glycol monobutyl ether ($C_4H_9OCH_2CH_2OH$) may include the formation of hydrogen peroxide (**H_2O_2**), as in Equation 3:

$C_4H_9OCH_2CH_2OH + 3O_2 \rightarrow 4CO_2 + 5H_2O + \mathbf{H_2O_2}$ (Eq. 3)

Note: **H_2O_2 (**oxidizing agent**)**

   d. Vinyl chloride and benzene are normally considered incompatible. If these substances come into contact, there is a potential for them to react with each other, leading to the production of harmful byproducts. Moreover, both substances are toxic and can pose health hazards, as in Equation 4.

$C_2H_3Cl + C_6H_6 \rightarrow C_6H_4{=}CH\text{-}Cl + \mathbf{H_2}$ **(Eq. 4)**

Note: H_2 (reducing agent)

7) New reactions that may emerge from the previous reactions:

   a. The reaction between vinyl chloride and hydrogen peroxides, as in Equation 5:

$C_2H_3Cl + H_2O_2 \rightarrow 2\ HCl + CO_2 + H_2O$ (Eq. 5)

   b. Phosgene ($COCl_2$) and benzene (C_6H_6) can react together in the presence of heat. However, it generally requires a catalyst, such as aluminum chloride ($AlCl_3$) or ferric chloride ($FeCl_3$), to proceed efficiently. If the reaction occurs, it could be described as in Equation 6:

$COCl_2 + C_6H_6 \rightarrow C_6H_5COCl + HCl$ (Eq. 6)

   c. Hydrogen is a reducing agent that can react with the atmosphere to produce "detonating gas", if the mixture of Hydrogen and air is outside the safe concentration range, between 4% and 75% H_2 by volume, the reaction can

occur quickly and with a large release of energy, leading to an explosion, as in Equation 7.

$$2\ H_2 + O_2 \rightarrow 2\ H_2O \quad \text{(Eq. 7)}$$

d. Propylene glycol ($C_3H_8O_2$) can react with hydrochloric acid (HCl) to form propylene gas. Propylene gas is flammable and can form explosive mixtures in the atmosphere. as in Equation 8:

$$C_3H_8O_2 + HCl \rightarrow C_3H_6 + H_2O + Cl^- \quad \text{(Eq. 8)}$$

e. Ethylene glycol monobutyl ether ($C_6H_{14}O_2$) can react with iron from the train itself (Fe) to produce iron(II) butoxide ($Fe(C_4H_9O)_2$) and hydrogen gas (H_2). If the reaction occurs under fire or in the presence of a heat source, it could potentially lead to a bigger fire or explosion, as in Equation 9.

$$2Fe + 2C_6H_{14}O_2 \rightarrow 2Fe(C_4H_9O)_2 + H_2 \quad \text{(Eq. 9)}$$

f. HCl will provoque acid rain.

g. $COCl_2$ (phosgene) is toxic and lethal to mammals, birds, fish, and other living organisms.

So, the situation at the derailment site required a highly skilled and experienced response team with proper training and equipment to manage the potential hazards safely. This type of team is not easy to find, and maybe it was not 100% available at the time. Following the previous observations, the situation at the derailment site was dangerous and complex. The presence of multiple chemical compounds that were prone to catching fire, such as vinyl chloride, benzene, and propylene glycol, created a significant hazard. The possibility for the formation of explosive mixtures with the chemicals and the air, possibly leading to a catastrophic explosion, increased the problem. The spill of a class 1A carcinogenic chemical and the creation of other toxic substances by side reactions made the case worse. Given the dynamics of the situation, there may not have been enough time to plan the best course of action, and any decision had to consider the evolving and potentially worsening circumstances.

3. CONCLUSIONS

The reasons for this derailment were unclear at the time of this publication. Under the limited amount of information available to the author, it looks reasonable to assume that the train crew was apparently operating under regulations and did not look guilty of misconduct. The personnel working to contain the situation followed the orders they received. The local population was the victim of a terrible derailment. Serious further investigations are necessary to find the real root causes of this derailment and prevent such a terrible disaster from happening again.

4. DECLARATIONS

5.1. Study Limitations

This note is limited to the sources consulted and the amount of information available at the moment of the research.

5.2. Acknowledgements

This text includes information generated by an AI language model, ChatGPT, which was trained by OpenAI and accessed on 01 March.

5.3. Funding source

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5.4. Competing Interests

The author declares that no potential conflict of interest exists in this publication.

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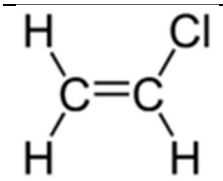
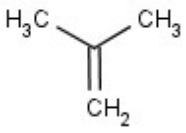
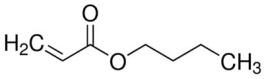
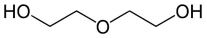
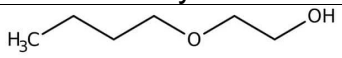
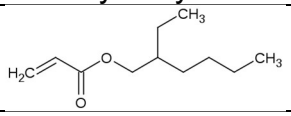
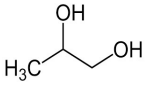
Table 1. *Chemicals present in the East Palestine derailment.*

			
Vinyl chloride.	Isobutylene	Butyl acrylate	Benzene
			
Diethylene glycol	ethylene glycol monobutyl ether	2-ethylhexyl acrylate	Propylene glycol