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WHY WAS VINYL CHLORIDE ON A TRAIN IN EAST PALESTINE, OHIO?

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- Inorganic chemistry created the chemical industry and remains important, but not particularly valued
- Scale remains the major source of competitive advantage in commodity chemicals
- Sustainability is multifaceted and complex with hidden interactions.



EAST PALESTINE, OHIO





- Norfolk Southern Railway train 32N derailed in East Palestine, Ohio on February 3, 2023
- a faulty wheel bearing caused the derailment
- fire ignited during the derailment and grew to involve 35 railcars
- derailed equipment included 11 tank cars carrying hazardous materials
 - 3 hazardous materials tank cars sustained mechanical and released flammable or combustible materials
 - 5 vinyl chloride (VCM) tank cars were not mechanically breached during the derailment
- VCM cars were explosively breached to initiate a vent and burn
- news outlets described the cargo as toxic, flammable and carcinogenic
- it was widely mentioned the burning created toxic materials

So why was VCM on the train?



BRIEF ASIDE



BNSF Railway freight train L-TWI8801-291

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TRAIN COMPARISON

- Vinyl chloride
 - flammable
 - toxic
 - carcinogenic
 - makes toxic materials when burned
 - HCI
 - CO₂
 - trace other stuff
 - fully-synthetic, unnatural
 - coproducts during production

- Ethanol
 - flammable
 - toxic
 - carcinogenic
 - makes toxic materials when burned
 - CO₂
 - trace other stuff
 - natural



VIEWS ON VINYL



PVC is single most environmentally damaging type of plastic.

PVC is one of the most toxic substances saturating our planet and its inhabitants. PVC contaminates humans and the environment throughout its lifecycle: during its production, use, and disposal.

Greenpeace







CARCINOGENIC



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- carcinogens are substances that may increase your risk of cancer.
 - Cleveland Clinic
- a carcinogen is a substance, organism or agent capable of causing cancer.
 - National Human Genome Institute
- a substance, organism, or agent capable of causing cancer
 - International Agency for Research on Cancer
- substances, mixtures, or exposure circumstances that are known or reasonably anticipated to cause cancer in humans
 - National Toxicology Program (NTP
- any substance that causes cancer.
 - National Cancer Institute

Vinyl Chloride Monomer(VCM)

Olin produced ~5 billion pounds/year World demand is 49 billion pounds Growth averages 4-5%



Source: Chemical Week product focus

USED TO MAKE POLYVINYL CHLORIDE (PVC)



- third largest polymer (by weight)
- infrastructure polymer
 - piping
 - siding
 - flooring
- main medical nolvmer

Vinyl chloride was on the train to make polyvinyl chloride.



- really bad material properties
 - brittle
 - low melting point
 - poor solvent resistance
- saving graces
 - cheap
 - takes filler well
 - solvent weldable
 - great with plasticizers
 - naturally flame retardant



PVC PRODUCTION: SUSPENSION POLYMERIZATION





https://www.nouryon.com/products/pvc-reactor-additives/

FREE RADICAL PROCESS





OxyVinyls Rail Route

from La Porte and Ingleside, TX to Pedricktown, NJ

Toledo

Pittshurg

Philadelphia

Fort Wayne

Vinyl chloride was on the train to provide feedstock for a polymer production facility far away from a monomer production facility.



887,400 pounds of VCM loaded at the Oxy Vinyls VCM plant in LaPorte, Texas



Phoenixville

King of

Going to Pedrickstown, NJ

Levittow

NOT THE FIRST TIME



- November 30, 2012 derailment on a moveable bridge in Paulsboro, New Jersey
- 3 VCM tank cars came to rest in Mantua Creek
- one was breached and released about 20,000 gallons of vinyl chloride



CHEMICAL INDUSTRY TECHNOLOGY WAVES

Inorganic

- mined materials
- electrochemical
- active reagents allow transformations

Functionalization

- use inorganics to transform organic substrates
- make dyes, solvents and drugs

Cellulosics

- use inorganics to transform natural materials
- partially synthetic polymers

Polymers

- took off with synthetic rubber
- continues today





WHAT IS INTEGRATION?







Linkage of mass and energy flows that create a significant advantage.







FOUNDATIONAL PILLARS OF THE MODERN CHEMICAL INDUSTRY

Electrochemical Chlor-Alkali

Steam Cracking









CHLOR-ALKALI





$Cl_2 + 2 NaOH \longrightarrow NaOCI + NaCI + H_2O$

• The oxidizing power of chlorine was what was desired.

• No net production of alkali







MEMBRANE CELLS





CO-PRODUCT PROCESSES



https://www.youtube.com/watch?v=YYkj2yYaGtU











Caustic Soda Chemistry and End Product Uses Products of the Chlorine Tree Caustic soda is a widely used industrial including in pulp and paper, detergents packaging, agriculture, environmental protection, water treatment, foodstuffs, healt textiles and in the chemical, construction and car industries.

> American[°] — Chemistry Council



ECU PRICING



icis.com/explore/resources/news/2019/03/21/10336962/insight-european-ecu-values-fall-to-the-lowest-level-since-2016/



ORGANOCHLORIDES









SUPERSOLVENTS



carbon tetrachloride	1,1,1-trichloroethane	trichlorethylene	tetrachlorethylene
carbon tet	1,1,1	tric	perchloroethylene
tet	TCA	TCE	perc
			PCE



CHEMICAL INDUSTRY SNAPSHOT



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ROUGH INDUSTRY MASS BALANCE



CHEMICAL TRANSFORMATION







ROUGH MASS BALANCE





IMPLICATIONS






CARBON FOOTPRINT OF INDUSTRY





GLOBAL CO2 EMISSIONS FROM INDUSTRY





RECENT INDUSTRY HISTORY









CRACKING COMPARISON





ALL REACTION PRODUCTS FIND USES





SCALE IS IMPORTANT





ORIGAMI DEMO





SCALE DEMO





DEMO МАТН





Power Law



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IMPACT OF SCALE TO CONTAIN SAME VOLUME





>2X material ~9X labor to construct







SCALE ALWAYS WINS



If you are moving mass around, scale reduces cost faster than experience.



ORGANOCHLORIDES





CHLORINE AS AN OXIDANT





CHLORINE AS AN OXIDANT









EPOXIDES





CHLOROHYDRIN CHEMISTRY

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Chlorohydrin Epichlorohydrin











Direct Oxidation Ethylene Oxide

 $\rightarrow + o_2 \rightarrow$



CHLOROHYDRIN CHEMISTRY

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titanium silicate catalyst

0.5 nm pores

suitable for packed bed reactor







CONVENTIONAL PRODUCTION











BREAKFAST OF CHAMPIONS



see Vonnegut's *Breakfast of Champions* or Pete Davidson's *The King of Staten Island*





Vinyl chloride was on the train because PVC production is the sink for chlorine that allows production of caustic soda.





CO-PRODUCT PROCESSES











Formation of Maillard reaction products



https://doi.org/10.3390/nu9080835

Denaturing Proteins

Vinyl chloride was on the train because of pretzels (and all the other uses of caustic necessary for modern life).





Lower Carbon Footprint



Source: Prepared from the survey report by Chem Systems



(Mcal/kg) 20 14.35 15.70 16.25 16.38 16.53 17.26 15 10.85 10 5 0 PVC HDPE LDPE PET Pp PS Expanded PS Source: Prepared from "A report on LCI data for petrochemical products", PWMI

Atom efficient – most inputs end up in the product



Energy Savings Over Lifetime



Long lifetimes during use in infrastructure.

Source: Prepared from "A document by the energy saving construction materials promotion center" within the Federation of Construction Material Industries, Japan


WHAT I HOPE I'VE LEFT YOU WITH

- Inorganic chemistry created the chemical industry and remains important, but not particularly valued vinyl and caustic are critical, just not particularly profitable chlorine has largely been replaced as an oxidant
- Scale remains the major source of competitive advantage in commodity chemicals

for undifferentiated materials, production cost is king and scale lowers production cost

• Sustainability is multifaceted and complex with hidden interactions.





INTEGRATED BIOREFINERY



Source: CIBE and CEFS (after British Sugar)

prokris.nl/production/



DISTRIBUTED MANUFACTURING



Resasco DE, Wang B, Sabatini D. Distributed processes for biomass conversion could aid UN Sustainable Development Goals. Nature Catalysis. 2018 Oct;1(10):731.







AG VERSUS CHEMICAL COMPARISON

