

Project Motivation

At Evonik, Process Engineers manually gather information from books and online sources to assess material compatibility. To ensure accuracy, a second Process Engineer verifies the generated compatibility matrices through a second-person verification (2PV) process. This is very time-consuming.

Project Goal: A dynamic program that automates the generation of Materials of Construction Matrices, streamlining compatibility assessments. The platform will also ensure security and accessibility, providing detailed records of edits, changes, and enhancements for traceability and reliability.

Data Scraping

- Our team was tasked with extracting data from numerous physical and online sources
- Each new source required a unique method of scraping the data. Examples of these different methods include:
 - Simply copy and pasting tables from a website to Excel
 - Writing a Python script to automate form submission to easily extract affinity for all chemical and material combinations
 - Using AI/online resources to read data from images of graphs
- After compiling all the data on an Excel sheet, we manually analyzed the list and made notes of chemicals that looked to be duplicates
- The duplicate chemicals were sent to our corporate partners for them to inform us which chemicals needed to be deleted, combined, or left separate

CHEMICAL COMPATIBILITY

Elastomer(Reverse) Lookup

Chemicals (Selected: Acetic Acid, 5%)

Acetaldehyde
Acetamide
Acetonitrile
Acetic Acid Amide
Acetic Acid Ethyl Ester
Acetic Acid, 20% to 80%
Acetic Acid, 5%
Acetic Acid, 85%
Acetic Acid, Glacial
Acetic Acid Methyl Ester
Acetic Aldehyde
Acetic Anhydride
Acetic Ester
Acetoacetic Acid
Acetol
Acetone

Elastomers		
Bakelite™ (Bakelite)	Unsatisfactory	🔴
Chloroprene (CR)	Satisfactory	🟢
Ethylene Propylene (EPDM)	Satisfactory	🟢
Fluorocarbon (FPM)	Satisfactory	🟢
Fluorocarbon (FKM)	Satisfactory	🟢
Fluorosilicone (FVMQ)	Fair	🟡
Hydrogenated Nitrile (HNBR)	Fair	🟡
Nitrile (NBR)	Fair	🟡
Perfluoroelastomer (FFKM)	Satisfactory	🟢
Polytetrafluoroethylene (PTFE)	No Data Available	🔴
Silicone (VMQ)	Satisfactory	🟢
Tetrafluoroethylene-Propylene (F2PM)	Satisfactory	🟢

Rating	Description	Volume Change	Comments	Code
Satisfactory	Little or no effect	< 10%	Elastomer may exhibit slight swelling and/or loss of physical properties under severe conditions	🟢
Fair	Possible loss of physical properties	10 - 20%	Elastomer may exhibit swelling in addition to a change in physical properties. May be suitable for static applications	🟡
Severe Effects	Noticeable change	20 - 40%	Elastomer exhibits a noticeable change in swelling and physical properties. Anticipate questionable performance in most applications.	🔴
Unsatisfactory	Excessive change	> 40%	Elastomer not suitable for service	🔴
N/A	Insufficient info	N/A	Insufficient information for rating	🔴

Backend

Initial Development

- Project initially as Excel-based, using scraped data stored in spreadsheets
- Identified limitations in scalability and functionality
- Consulted mentors for feedback and guidance
- Pivoted to a web-based solution with their support
- Migrated raw data to Microsoft SQL Server for:
 - Improved data security
 - Better scalability
 - Enhanced data management and reliability

Updated Solution

After receiving mentor approval, we built a full-stack web app using React for the front end and JavaScript/TypeScript for the back end. MySQL handled data flow between the front end and our SQL Server database.

- Backend Tehcnologies:** JavaScript, TypeScript, MySQL SQL Server Management Studio (used for storing data)

Frontend

The Evonik Matrix Manager is a web app for creating and managing chemical-metal affinity matrices. It includes secure, role-based login, with dashboards tailored to user roles—enabling matrix creation, viewing, and, for admins, data and access management.

- Frontend Technologies:** TypeScript, React, Tailwind CSS, HTML, CSS, JavaScript

Edit Chemical-Material Affinity Master Data

Welcome, John Doe. As an admin, you can edit the chemical and material master data.

Chemicals

Materials

Chemical List

Import Chemicals from CSV

+ Add Chemical

CSV format: Name,Formula (header row required)

ID	Name	Formula	Actions
1	Hydrogen Peroxide	H2O2	✎ 🗑
2	Sulfuric Acid	H2SO4	✎ 🗑
3	Nitric Acid	HNO3	✎ 🗑
4	Sodium Hydroxide	NaOH	✎ 🗑
5	Hydrochloric Acid	HCl	✎ 🗑

Conclusion

After many phases we are proud of the work we have done and the final product, including:

- Automating a manual, Excel-based process with a full-stack web app
- Improving efficiency, scalability, security, and accessibility
- Resolving data inconsistencies through cleaning and standardization
- Enhancing accuracy of chemical compatibility assessments
- Supporting Evonik's focus on innovation and sustainability

Chemical	Material	Result
Acetaldehyde	12614 Leadloy Carbon Steel	NR _g
1-Butene 2-Ethyl	Buna-N/ Nitrile	U
Coffee	Aluminum	
Fuel Oil	304 Stainless Steel	A _g
1 - Chlorol 1 Nitro Ethane	Chloropene Cr	U

Chemicals	12614 Leadlo	2024-T4 Alum	302 Stainless
Cacao Butter	Chemical not	Chemical not	Chemical not
Fuel Oil	Q _g	U	U
Acetaldehyde	NR _g	U	A _g °C ₄
Chromic Acid 10%	U	U	U
0 - Chloronaphthalene	U	U	U

Future Work

We have many ideas for future improvements and features that could further enhance this project.

- Implement advanced search and filter options for matrix data
- Add support for visualizing chemical-metal interactions with charts or heatmaps
- Integrate user feedback features to improve usability and accuracy
- Expand compatibility data sources for broader chemical coverage
- Explore machine learning models to predict unknown compatibilities
- Enhance mobile responsiveness and cross-platform accessibility

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