OVERVIEW

CAS Custom Services℠

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American Chemical Society

Who we are

About CAS

- Founded in 1907 as a division of the American Chemical Society
- Our experts collect, harmonize, organize, and connect the world's scientific information
- Our proprietary ontologies, lexicons, and thesauri enable and accelerate insights
- We develop and license technologies to access our content

CAS DATA:

- CAS Registry Numbers®
- Chemical structures and reactions
- Physicochemical properties
- Spectra
- Analytical methods
- Toxicological and regulatory data (the GHS)
- Commercial sources
- Global patents and published research
- Life sciences

Over
1,000
experts who speak
50
languages

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CAS Custom Services℠ Core Capabilities

Aligned to your scientific information journey

Content Management: Internal Data Discovery	Knowledge Management: Data Design	Prediction: AI	Data-Enabled Risk Management	Search
Do you know what you know? Don't waste knowledge and past investments	*Your research is generating more data than ever, what to do about it*	*AI should excite you, not concern you. Make content advances work for you*	*Sci-information doesn't just help innovate, it can also protect your business*	*Sometimes we all need an extra set of experienced eyes or additional help*
Digitization	Substance Registry	Training Data Sets (Algorithm Development)	Responsible Synthesis Design	IP Custom Search - Landscape - State of the Art - Freedom to Operate - Novelty - Pre-Patent Examination - Written Opinions
Data Extraction	Domain Modeling & Governance	Custom AI Data Curation	Substance Supply Chain Analysis	
Data Normalization	Structure Normalization	AI Data Support	Substance Regulatory Status & Safety	
Taxonomies	Data Migration	Retrieval Augmented Generation (RAG) Solutions	Toxicology Literature Review	
System Search	Content System Audit	AI-Based Research Area Assessments	Commercial Sourcing	
	External Data Connection		Alternatives Analysis	

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Case Study | Increase Reactor Utilization

Identify new product candidates for under-utilized manufacturing assets

Objectives

- **Increase asset utilization**
- Identify potential products for an under-utilized chemical reactor
- Consider existing raw materials only

Outcomes

- Identified **201 new product candidates**
- Provided industry application insight
- **Asset utilization increased**

Approach

1 Identify Raw Materials and Process Constraints

- Raw materials on-hand
- Allowed solvents, reagents, and catalysts
- Process temperature and pressure

2 Identify Reaction Candidates

- Input substance reactant role
- Reaction conditions: temperature and pressure
- Availability of additional reactants

3 Identify Product Candidates

- Synthetic Pathways: reactions, yields, aromaticity, atoms
- Physical Properties: LogP, temp, solubility, molecule size
- Sustainability: regulatory and transportation
- Commercial: availability, supplier count, and market price
- IPC: indicator of industry application

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CHEMICAL SUPPLY CHAIN MAPPING

Approach and recent work

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Supply chain impact analysis

- **Commodity price changes**: material and product cost impacts
- **Material sourcing**: natural, synthetic, greener production pathways

Develop	Models – Predicting financial impacts of pricing changes from commodities / raw materials – Tracking origination of ingredients
Understand	Purchased materials and volumes
Trace	Preparation steps for purchased materials – Reactions, reagents, raw materials
Provide	‘Map’ tracing purchased materials back to a commodity or raw materials

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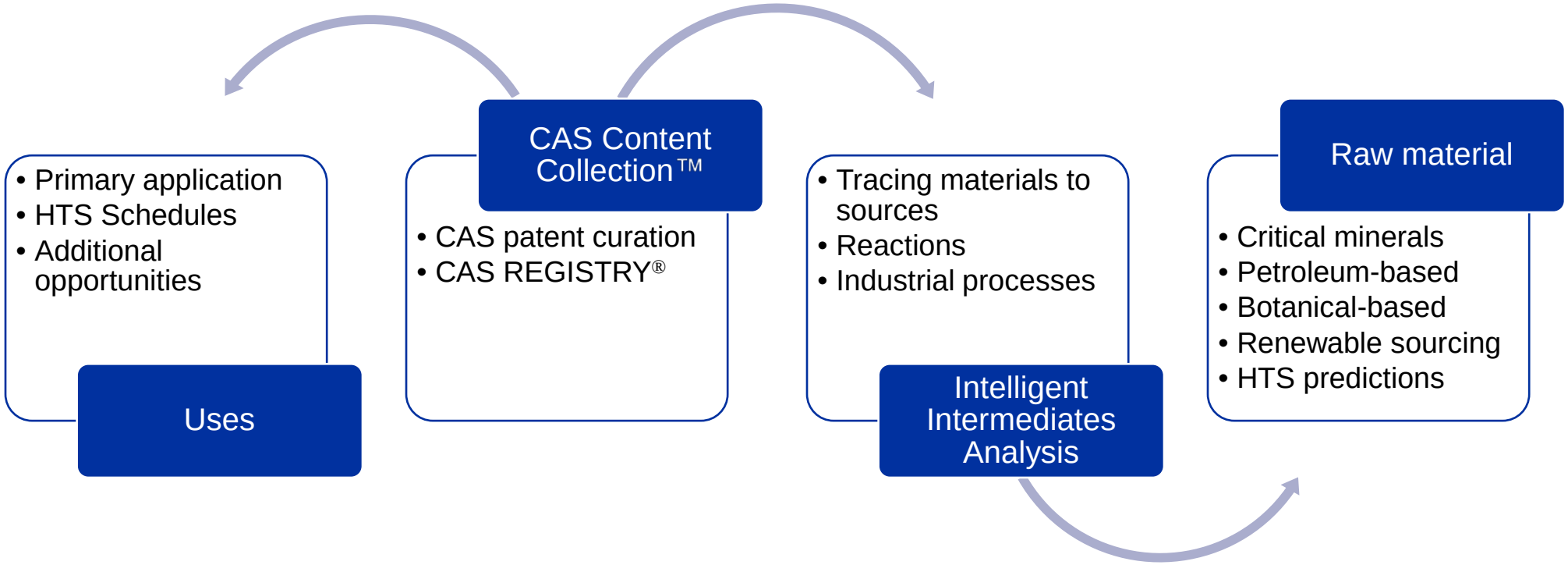
Supply chain mapping capabilities



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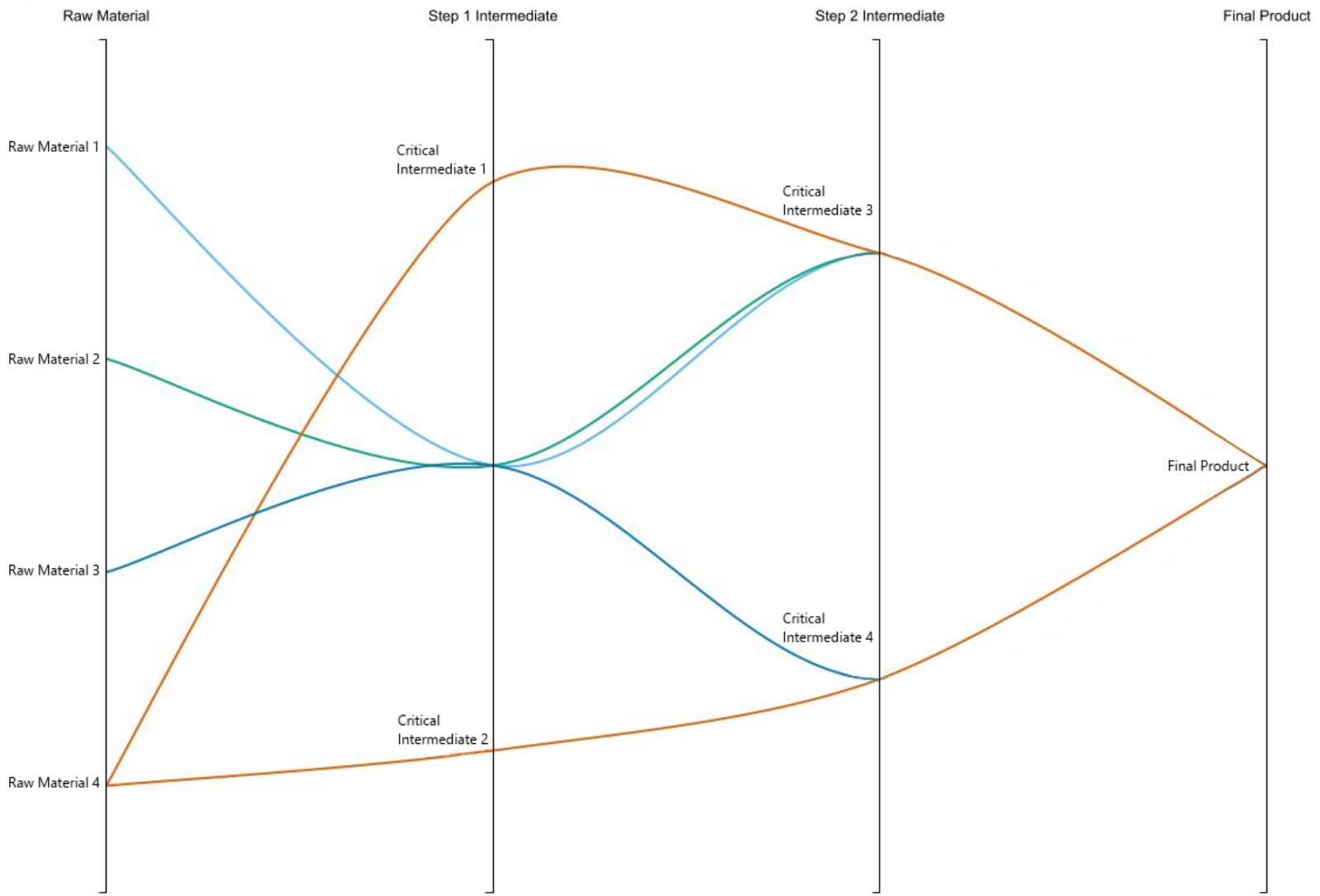
Interpreting the pathway



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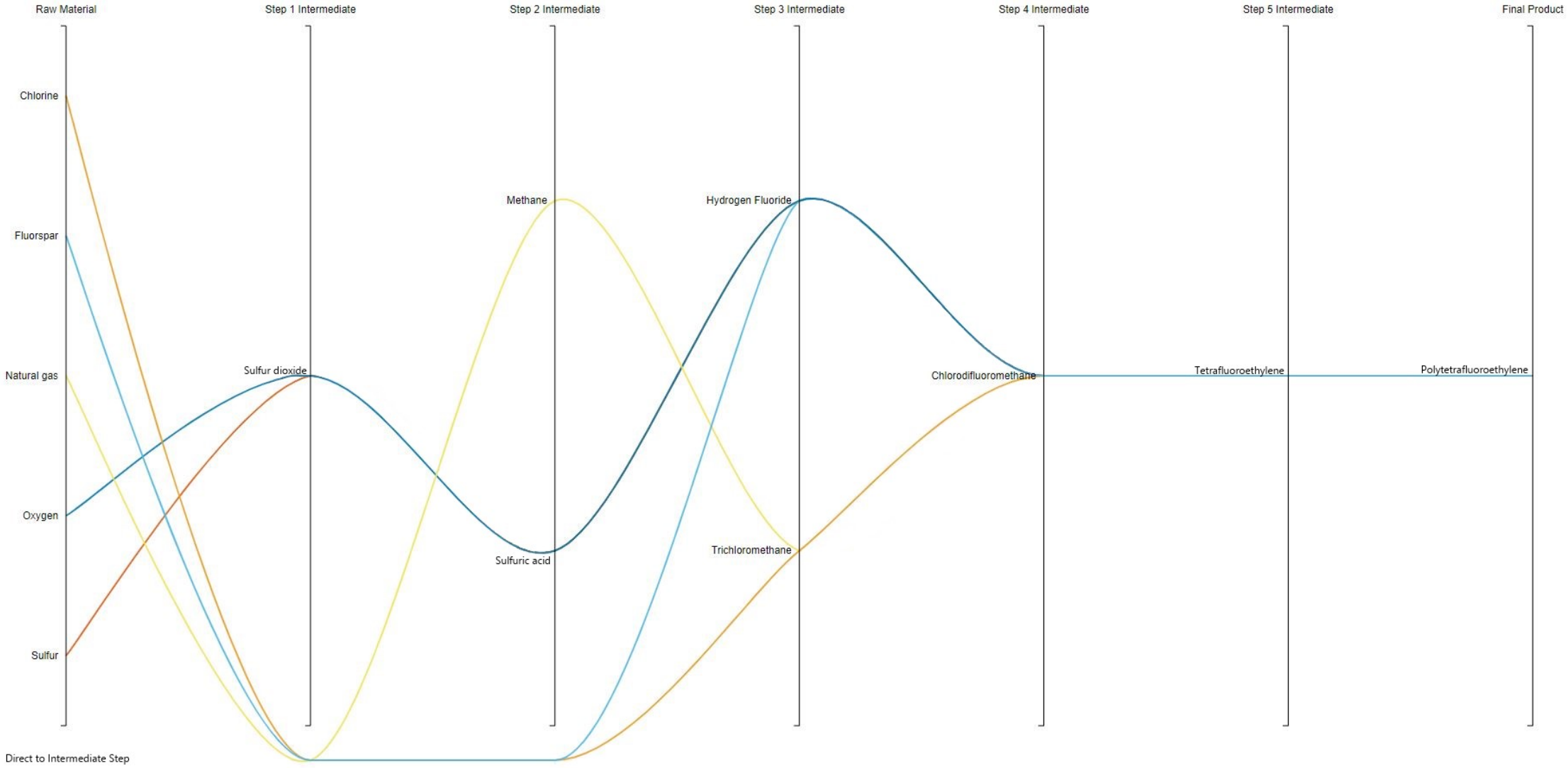
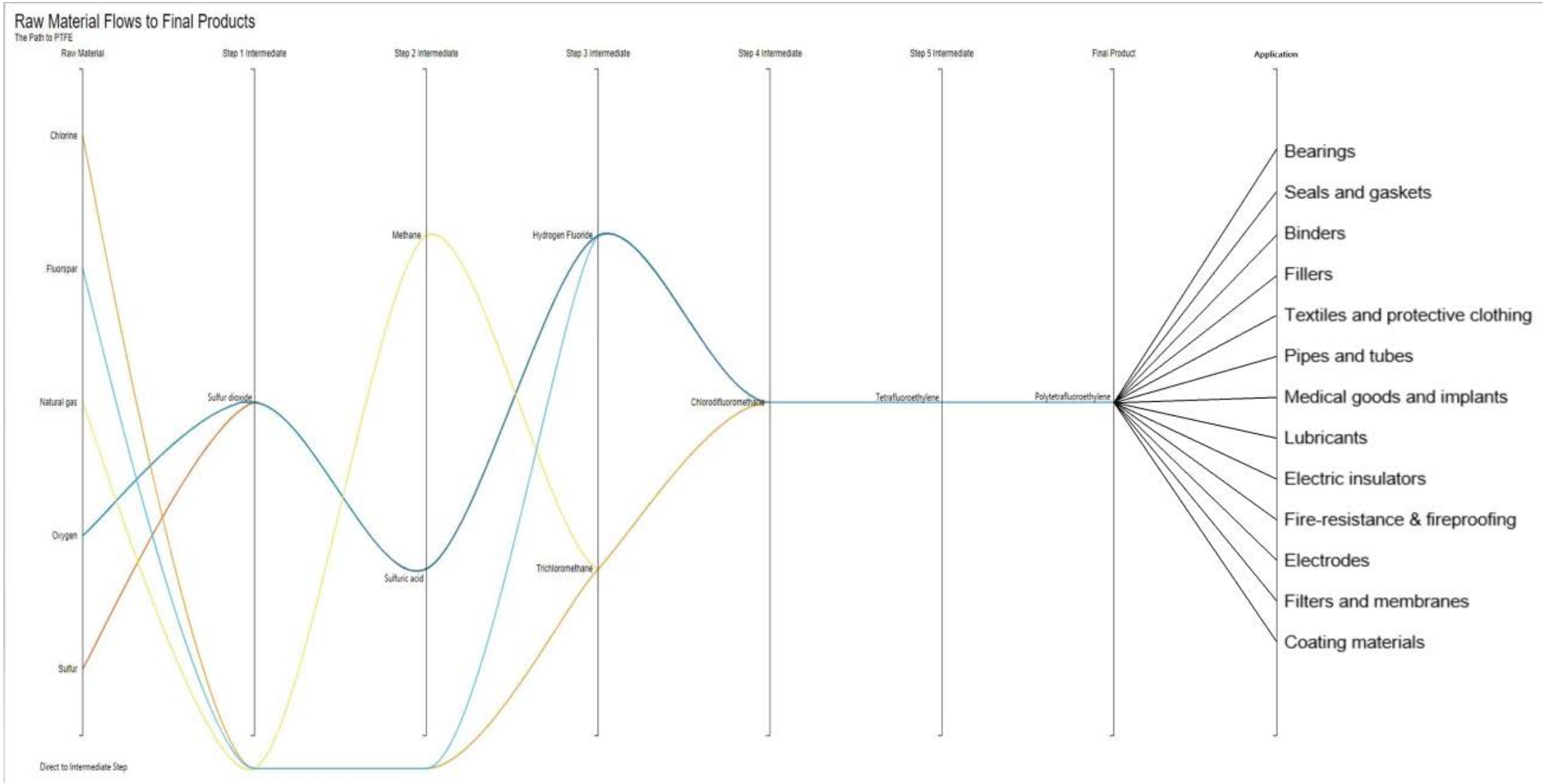
Raw Material Flows to Final Products

The Path to PTFE



Production and applications



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Raw Material Flows to Final Products

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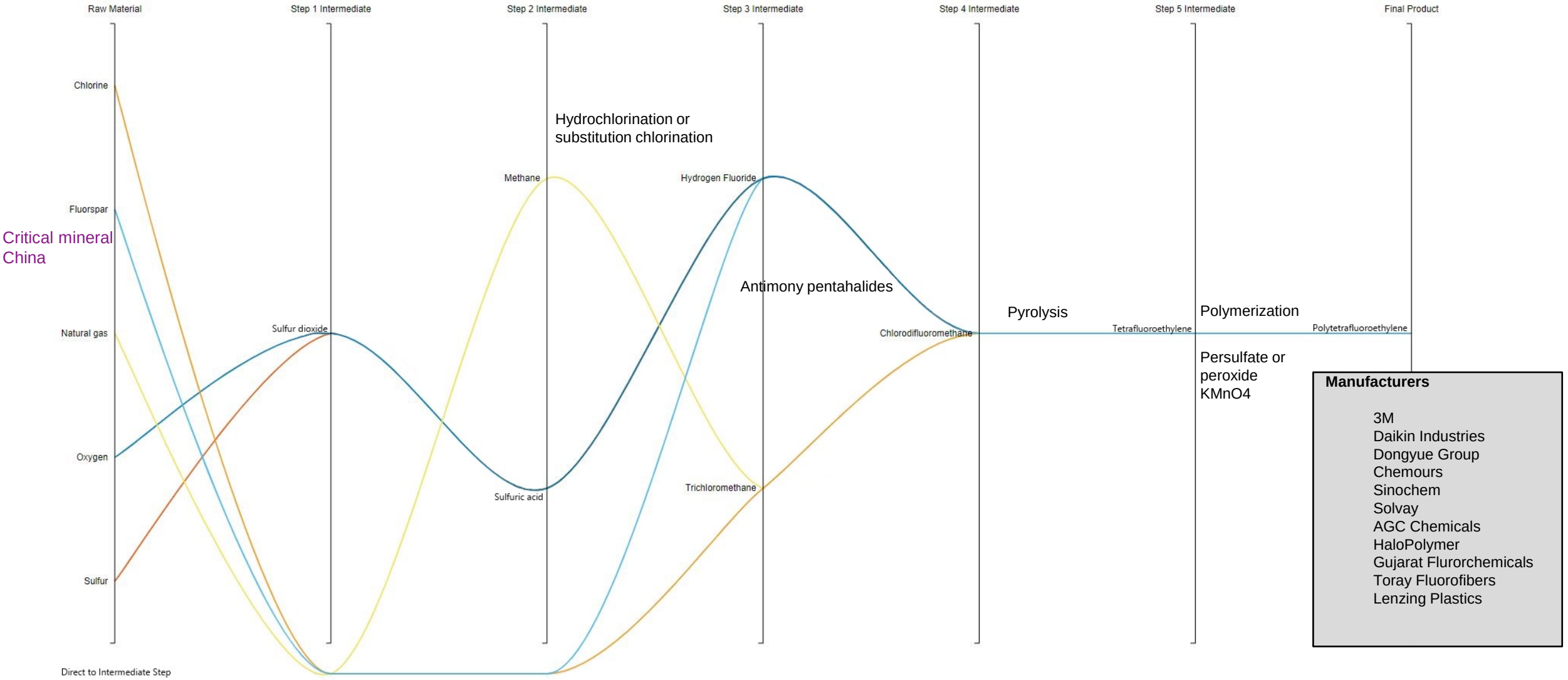

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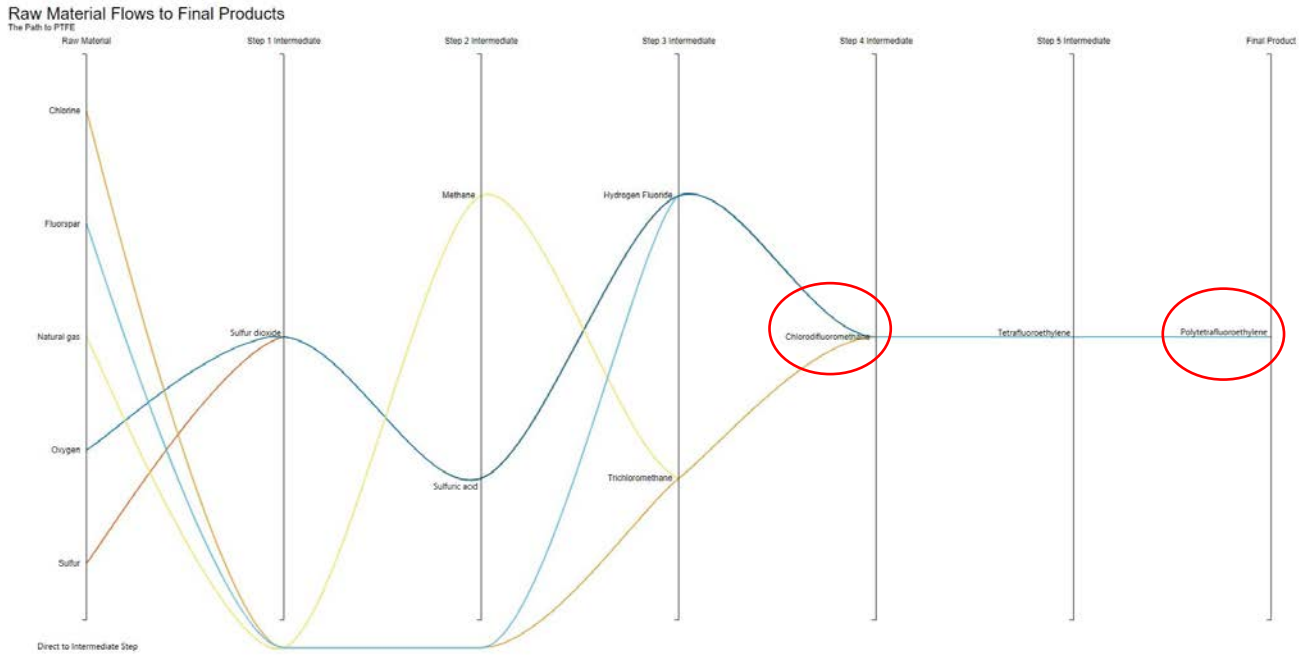
PFAS in the supply chain

OECD’s PFAS classifications

Chemical Name	CAS RN	Classification	Is PFAS by OECD Definition
Chlorodifluoromethane	75-45-6	Intermediate	Noted Exception
Polytetrafluoroethane	9002-84-0	Final Product	Yes

PFASs are defined as fluorinated substances that contain at least one **fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)**, i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group ($-CF_3$) or a perfluorinated methylene group ($-CF_2-$) is a PFAS.



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HTS MAPPING

Identifying chemicals corresponding to tariff codes

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HTS Mapping Example

Many substances may be assigned the same tariff code

US Harmonized Tariff Schedule

2929.90.50		Other.....
	15	*N,N*-Dialkyl (methyl, ethyl, *n*-propyl or isopropyl) phosphoramidic dihalides: *N,N*-Dimethylphosphoramidic dichloride.....
	18	Other.....
	20	Dialkyl (methyl, ethyl, *n*-propyl or isopropyl)-*N,N*-dialkyl (methyl, ethyl, *n*-propyl or isopropyl) phosphoramidates.....

Example CAS RNs

597-07-9
848216-05-7
676340-60-6
122081-90-7
848216-05-7
65659-19-0
848216-06-8
848216-07-9
676340-60-6
848216-06-8
90272-62-1
848216-08-0
122081-90-7
848216-07-9
848216-08-0
170275-46-4
2404-03-7
53279-98-4

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ALTERNATIVES ANALYSIS

Identifying candidate substitutes to replace chemicals of concern

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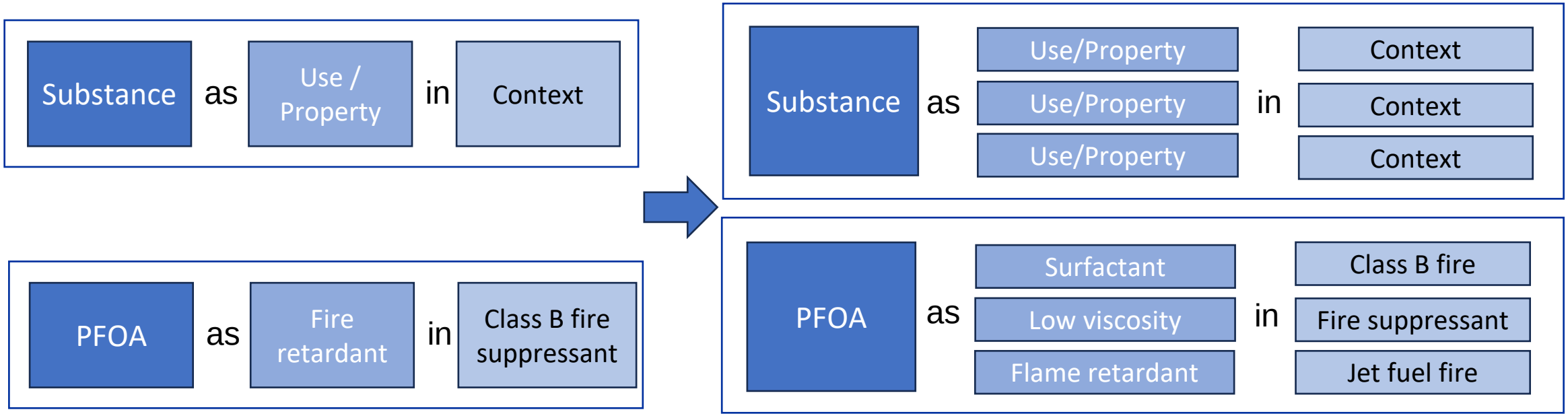
Alternatives analysis

- Alternatives identification
  - Select incumbent substances for replacement, or
  - Begin with a known incumbent substance
- Outcome: List of potential candidate substitutes for further downselection and testing

Alternatives analysis

Discovery of uses



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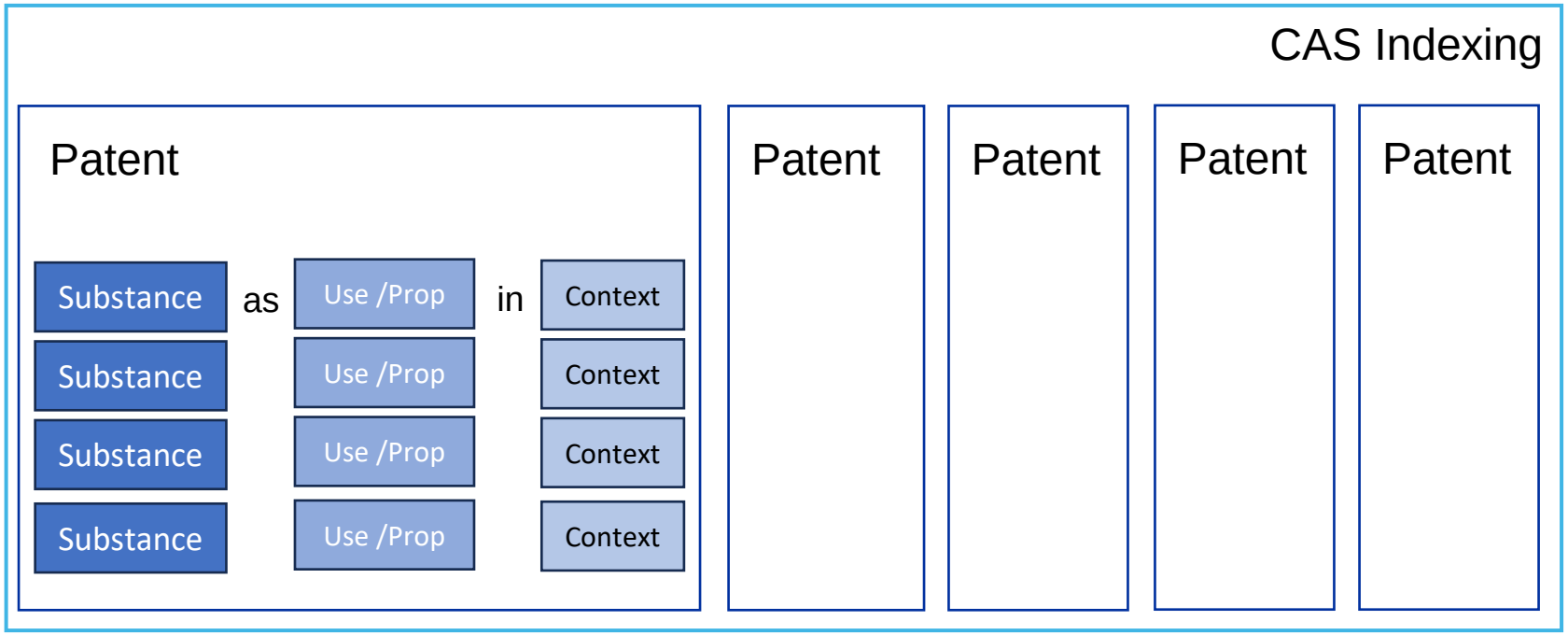
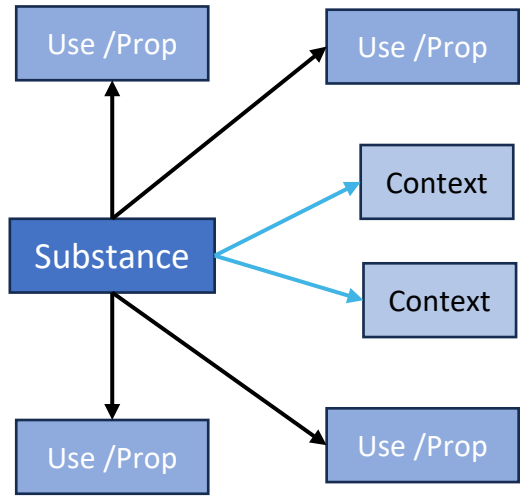
Proximity network analysis





Identify most relevant CAS substances as alternates

- Has the most of the same or closely related properties (impact modifier vs. toughening agent)
- Correlate on needed properties over known use

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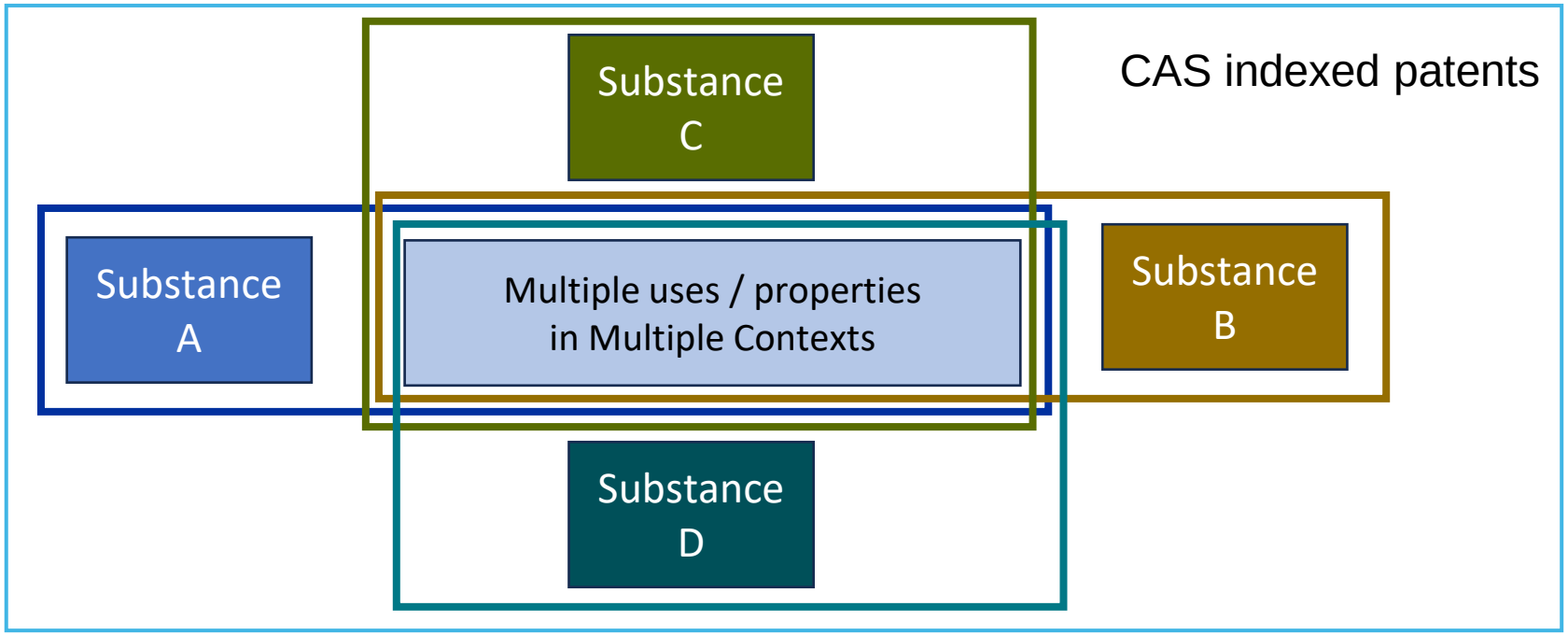
Proximity network analysis



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Thank you

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