Connecting Data to Decisions

How does a process development chemist initiate, assess, and evaluate a green chemistry approach to improve its sustainability goals?

As chemists (and scientists in general), the process's viability is measured empirically with a designed experiment. Viability is measured differently for each process.

For some processes, it might be how waterproof a jacket is; for another, it might be how clean a surface is.

"Data" is what we use to determine this viability, and "modeling" that data is how we know which conditions to select in our decision-making process.

How To Drive Decisions in Green Chemistry

- No one is “against” green chemistry
- Many Stakeholders prefer to make data-driven decision.
- There is no single best solution
- There is necessarily some give and take in any selection

Optimization: understanding trade-offs

Process development chemists and others on the bench are engaged in identifying and communicating trade-offs.

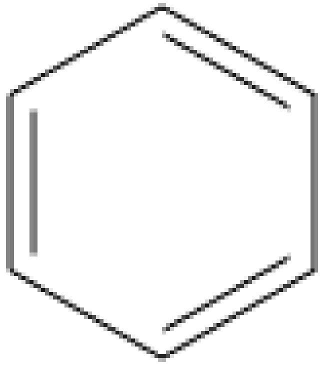
A Fictional Example

Technotron

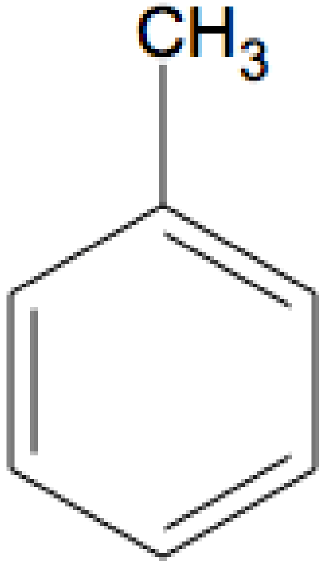
EnviroTRON

Greener Than Technotron

Environtron is seeking a new greener solvent



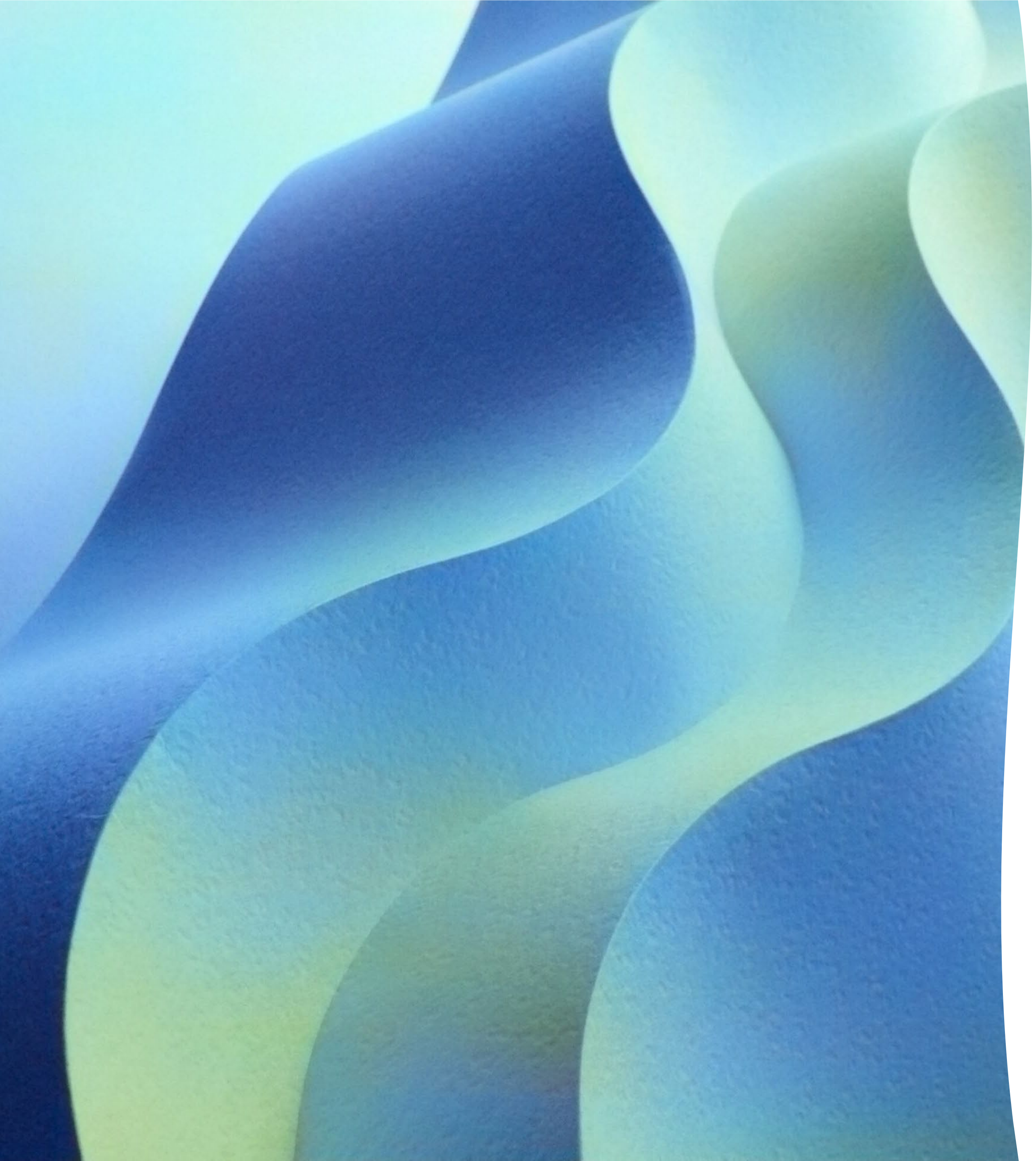
Benzene
Carcinogenic



Toluene
Alternative Candidate

Envirotron starts to wonder if they made the best choice

	Benzene	Toluene
Toxicity (Carcinogenicity)	Extreme	None
Material Cost	$265,000/ year	$703,000/year
Toxicity (reproductive?)	No Data	No Data
Material Scrap Cost	$200,000/year	$800,000/year
Processing time cost	Standard	20% longer
Environmental Impact	Low	Low



A new approach

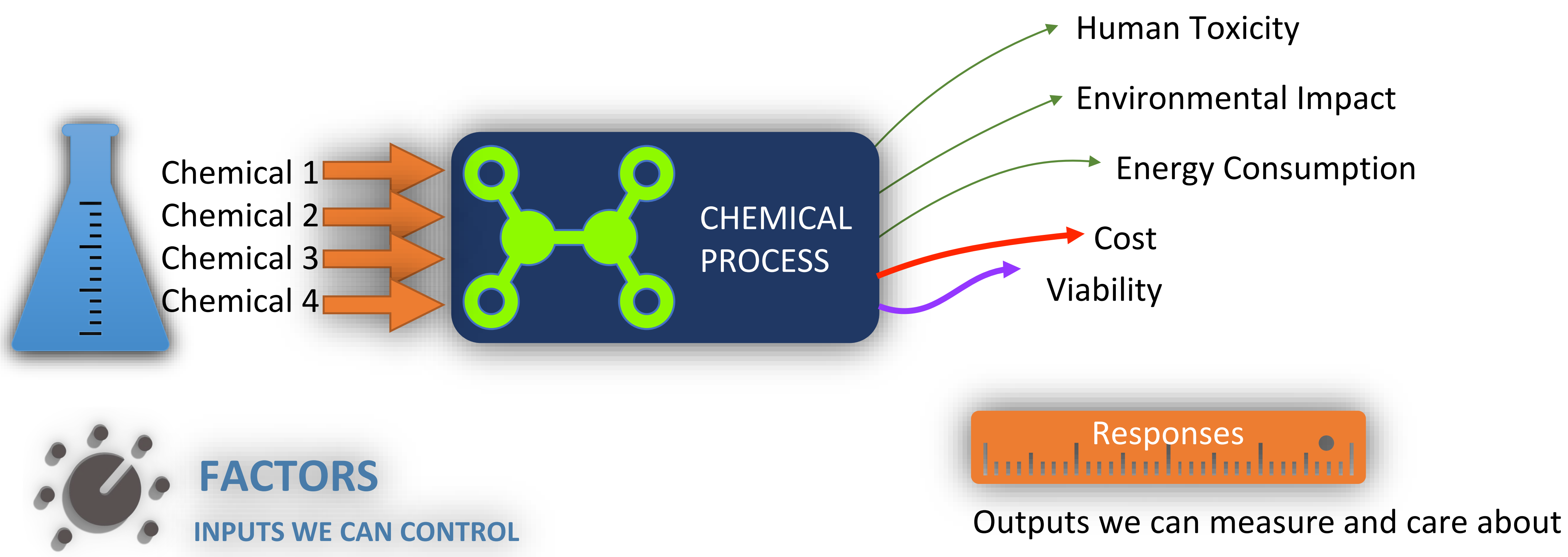
CREATE A BUSINESS CASE AND A TECHNICAL CASE

BUILD A MODEL BASED ON RESEARCHED DATA AND EXPERIMENTAL DATA

Build A Model

The link between data and decision is a model.

"All models are wrong, but some are useful"- George Box



UNDERSTAND YOUR GOALS BY MAKING A RESPONSE TABLE

Response Name	Goal	Lower Limit	Upper Limit	Importance
Acute Toxicity	Minimize	1	4	10
Birth Defect	Minimize	1	4	10
Reproductive Harm	Minimize	1	4	8
Endocrine Disruption	Minimize	1	4	7
Cancer	Minimize	1	4	10
Brain/Nervous System Harm	Minimize	1	4	8
Persistant Bioaccumulative	Minimize	1	4	5
Flammability	Minimize	1	4	2
Aquatic Ecosystem Harm	Minimize	1	4	2
Land Ecosystem harm	Minimize	1	4	1
Cost ($/gallon)	Minimize	2	20	7
Viability (% parts pass)	Maximize	0	100	10

IDENTIFY WHAT CHEMICALS YOU MAY WANT TO USE. THESE ARE YOUR FACTORS

Factors

Add Factor | Remove | Add N Factors 1

Name	Role	Changes	Values	
Benzene	Continuous	Easy	0	100
Toluene	Continuous	Easy	0	100
Xylene	Continuous	Easy	0	100
Phenol	Continuous	Easy	0	100

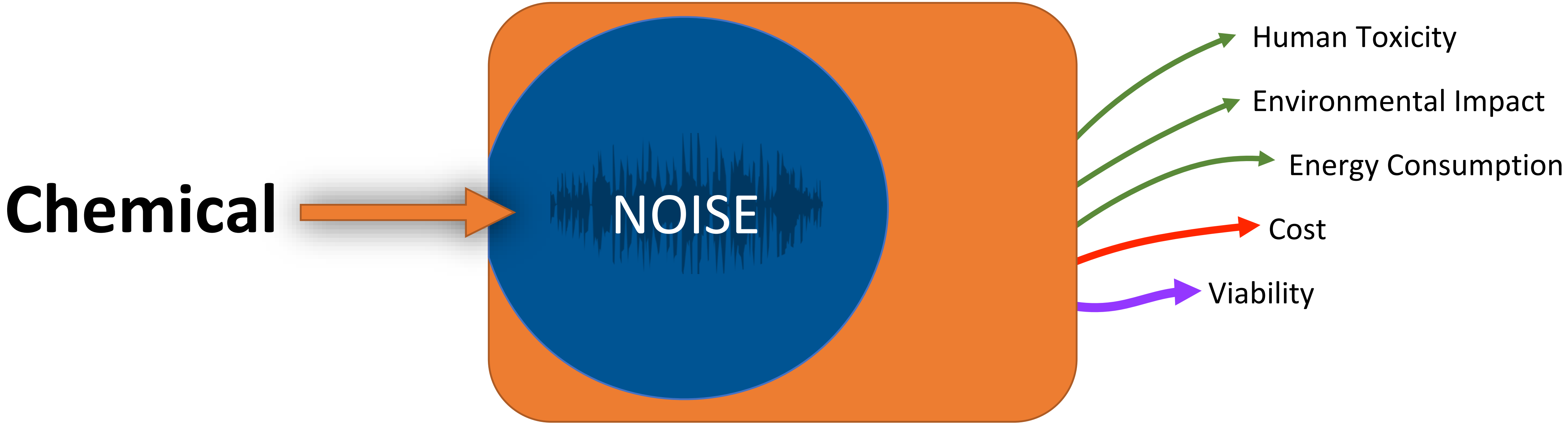
COLLECT THE DATA YOU CAN FROM RESEARCH AND GET THE REST BY RUNNING EXPERIMENTS

	Benzene	Toluene	Xylene	Phenol	Acute ...	Birt h...	Repro ductiv...	Endocrine ...	Cancer	Brain/N ervous...	Persistant ...	Flamma bility	Aquati c...	Land ...	Cost ($/ga...	Viability (% parts...
1	0.5	0.5	0	0	3	4	4	3	2.5	3	1	4	3	3	8	90
2	0.5	0	0.5	0	3	3.5	4	3	2.5	3	1.5	3.5	3	3	9	95
3	0	0	0	1	3	3	4	3	3	3	3	3	4	3	15	50
4	0	0.5	0	0.5	3	3.5	4	3	2	3	2	3.5	3.5	3	12.5	65
5	0.5	0	0	0.5	3	3.5	4	3	3.5	3	2	3.5	3.5	3	10.5	75
6	0	1	0	0	3	4	4	3	1	3	1	4	3	3	10	80
7	0	0.5	0.5	0	3	3.5	4	3	1	3	1.5	3.5	3	3	11	85
8	0	0	0.5	0.5	3	3	4	3	2	3	2.5	3	3.5	3	13.5	70
9	0	0	0	1	3	3	4	3	3	3	3	3	4	3	15	50
10	1	0	0	0	3	4	4	3	4	3	1	4	3	3	6	100
11	0	1	0	0	3	4	4	3	1	3	1	4	3	3	10	80
12	0	0	1	0	3	3	4	3	1	3	2	3	3	3	12	90

Cost Data

Hazard Data

Viability Data



Understanding Noise

We have more trust in signals that are greater than the noise

Understanding the Model

The link between data and decision is a model.

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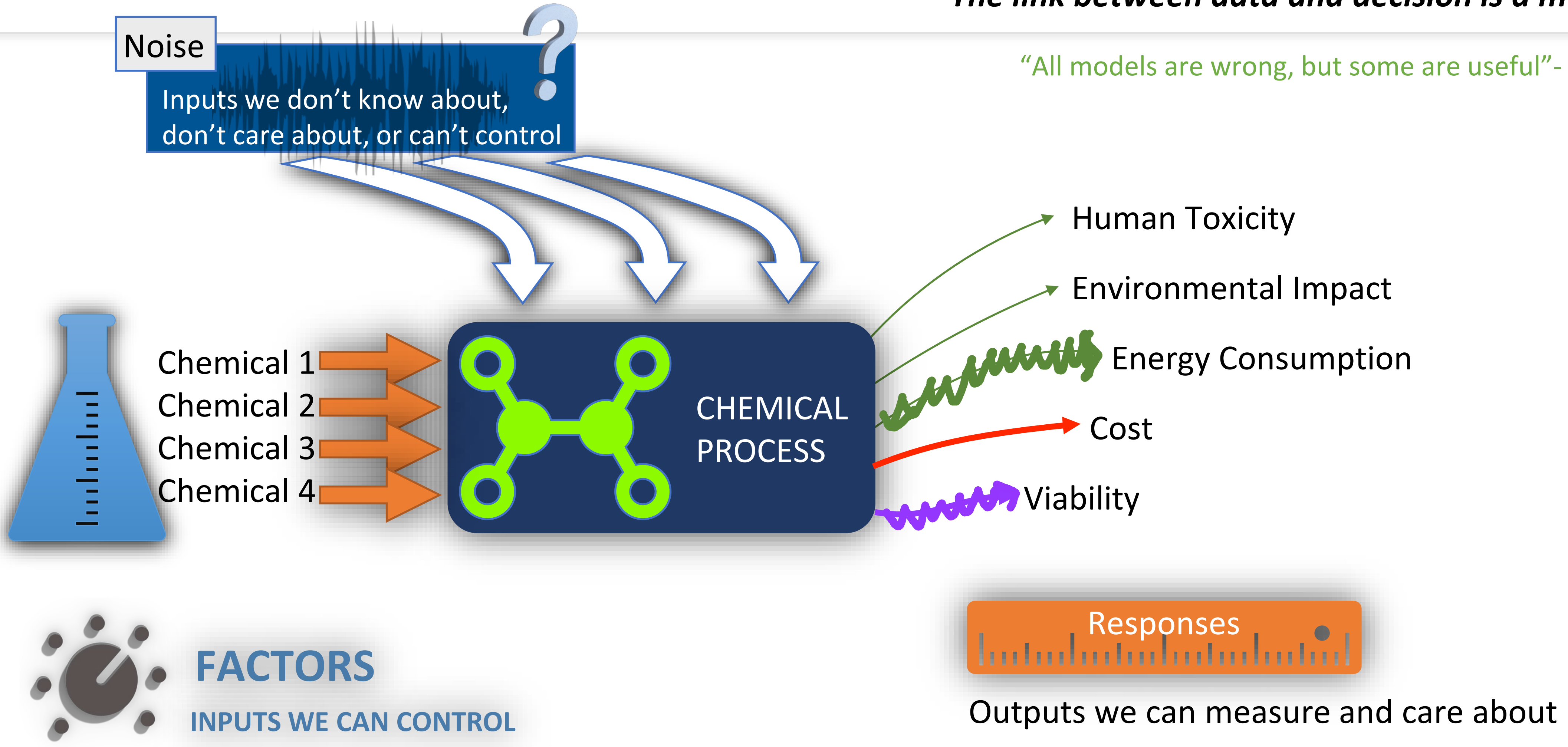
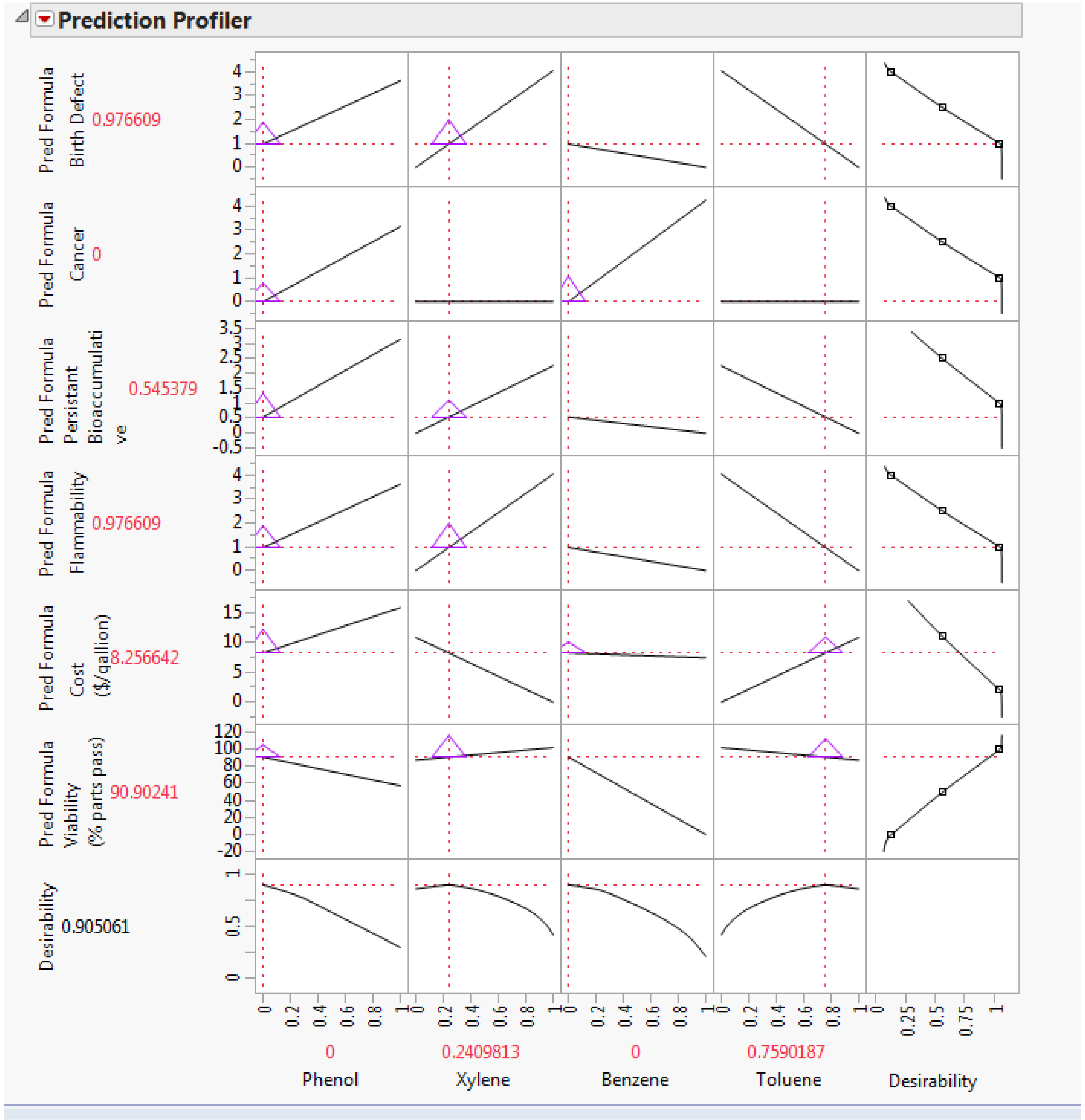
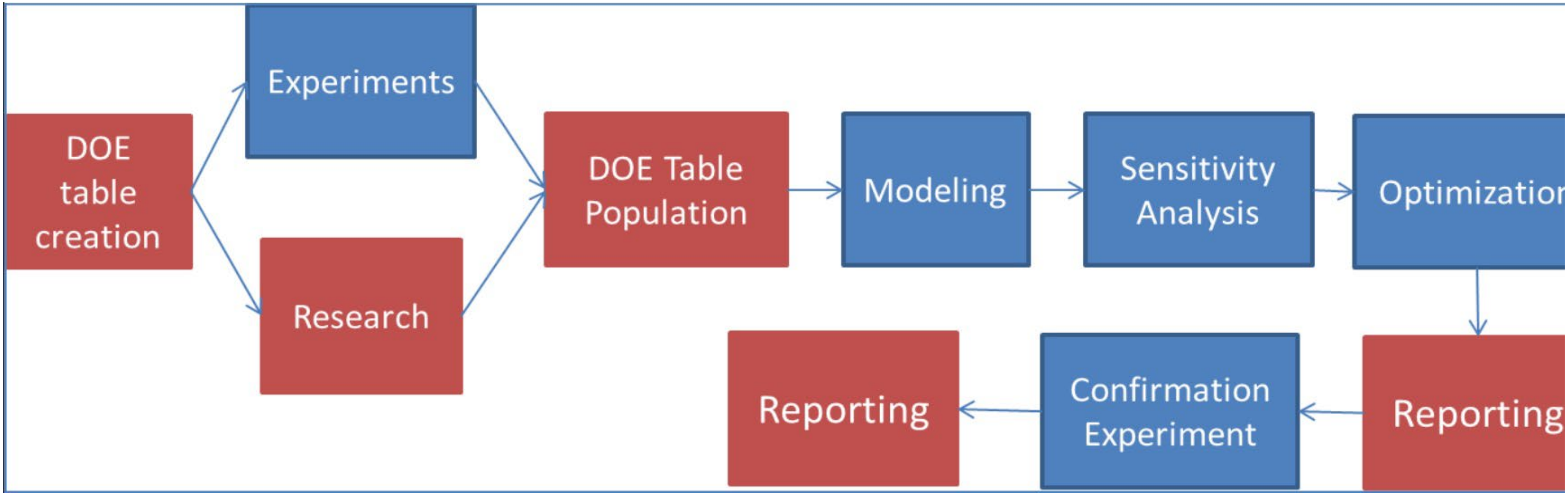


Create the Model and View Profiler





There are a few more steps

We still need to report the finding and then run confirmations experiments

Everyone Gets Some Green!