Getting the Chemistry Right

(well closer...)

Uncertainty and Regionalization approaches to enhance plastics data in LCA

Data Challenges Today:

Plastics Are Missing Additives

Between .01-70% of nt wt excluded from plastics data

Energy & Heat System Limitations

Not always representative of sourcing behaviors

How does including additive data in plastic conversion processes affect the uncertainty of the study?

Research Questions:

What are the effects of regionalizing the energy and heat systems to more accurately reflect production practices?

EVIL PLAN:

- Add additives and their uncertainties to plastic conversion data
- Update polymer content to reflect additive presence based on scenarios
- Propagate the uncertainty
- Replace the energy systems with both energy mixes and future energy mixes from the region desired
- Make it so.....

Should we regionalize every single electricity consumption?

Expected Challenges:

... until the screwdriver used to assemble the car?

We would like to regionalize only the 2nd or 3rd supply chain level...

It was identified how to do but it is time consuming.

COMPROMISE

Excluding Asia from sourcing

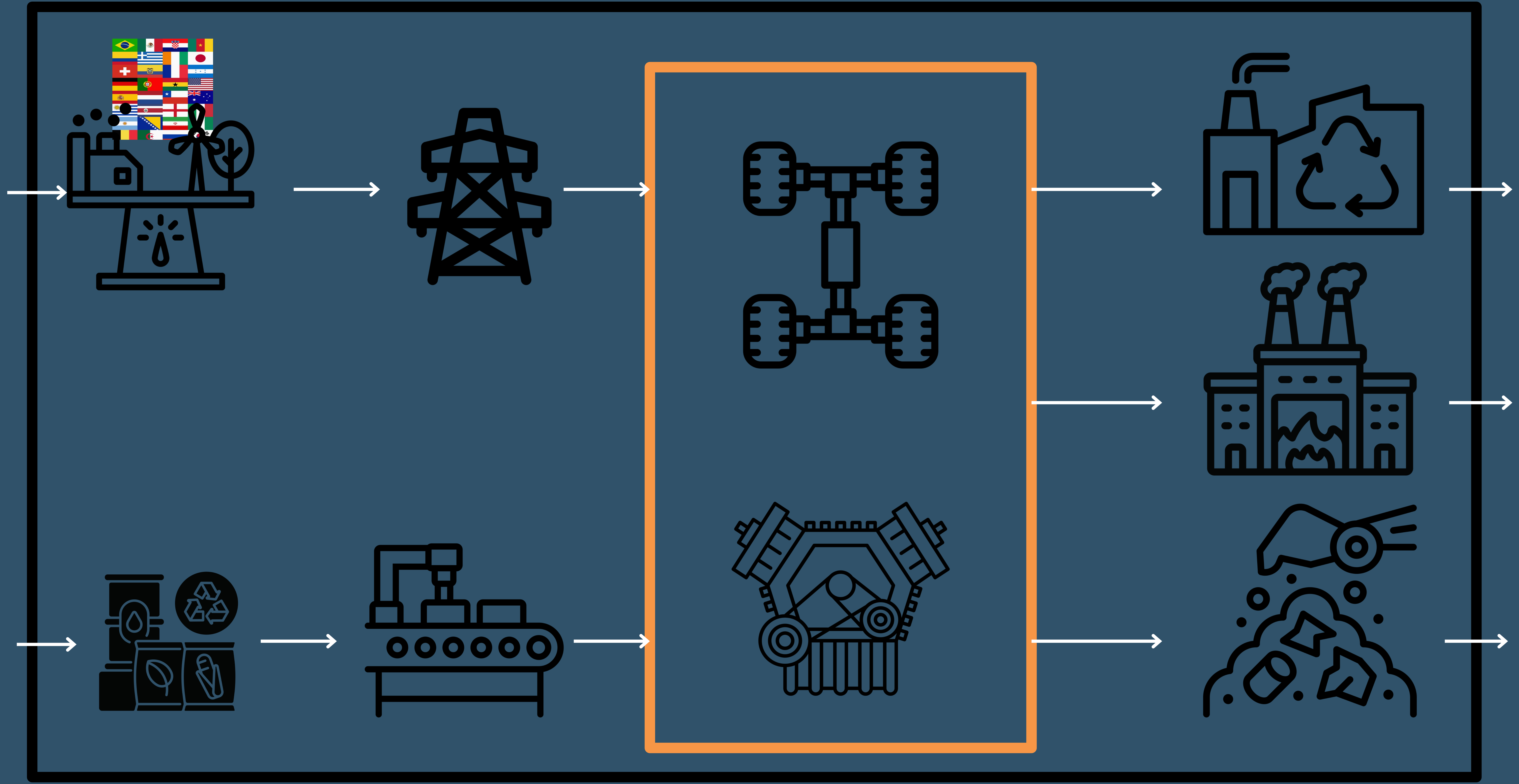
= relocating in DE all the Asian electricity consumption

Functional Unit:

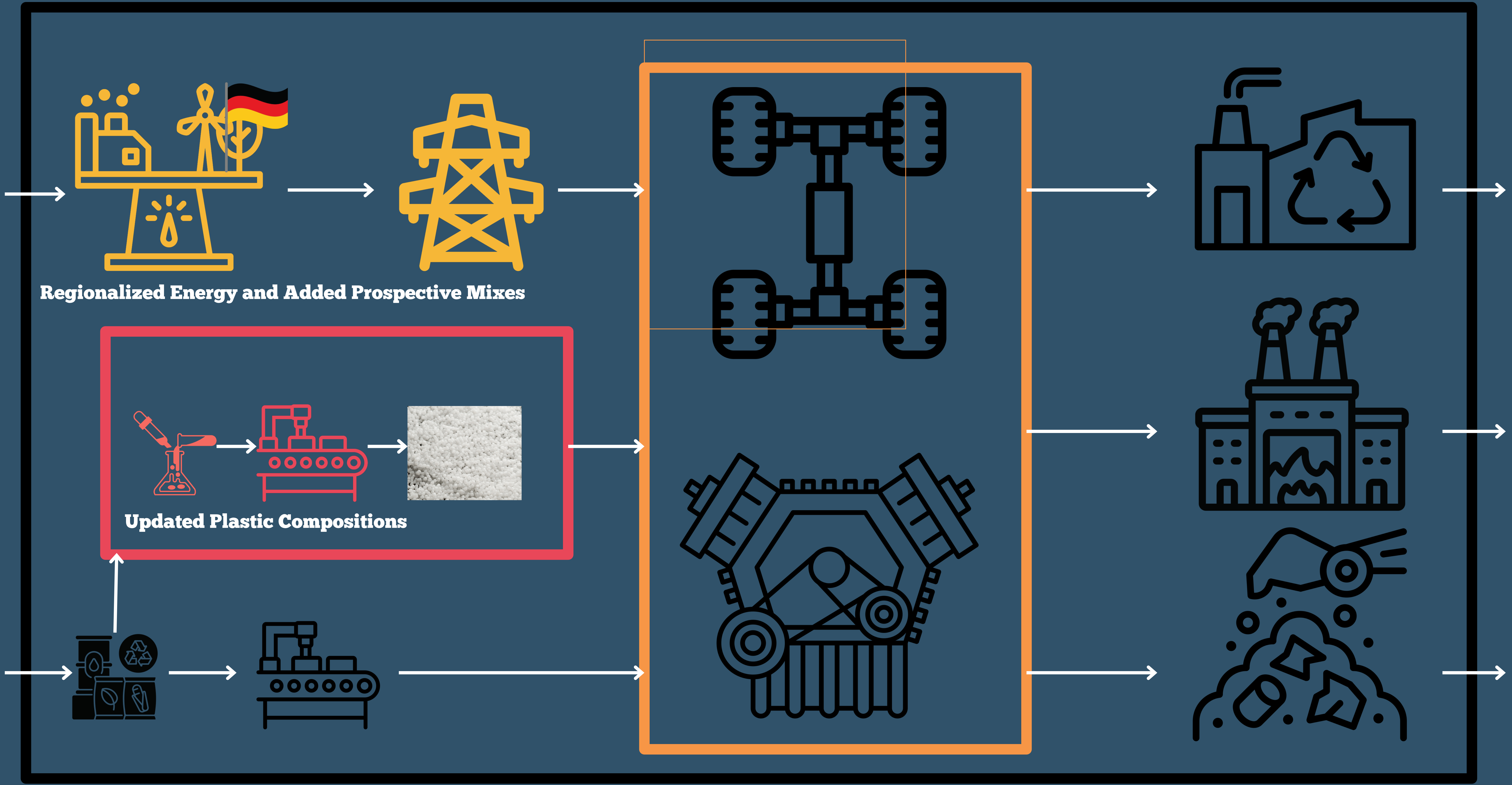
Case Study:

Production of 1 Electric Vehicle, without battery, in DE

Produced between the years of 2020-2030

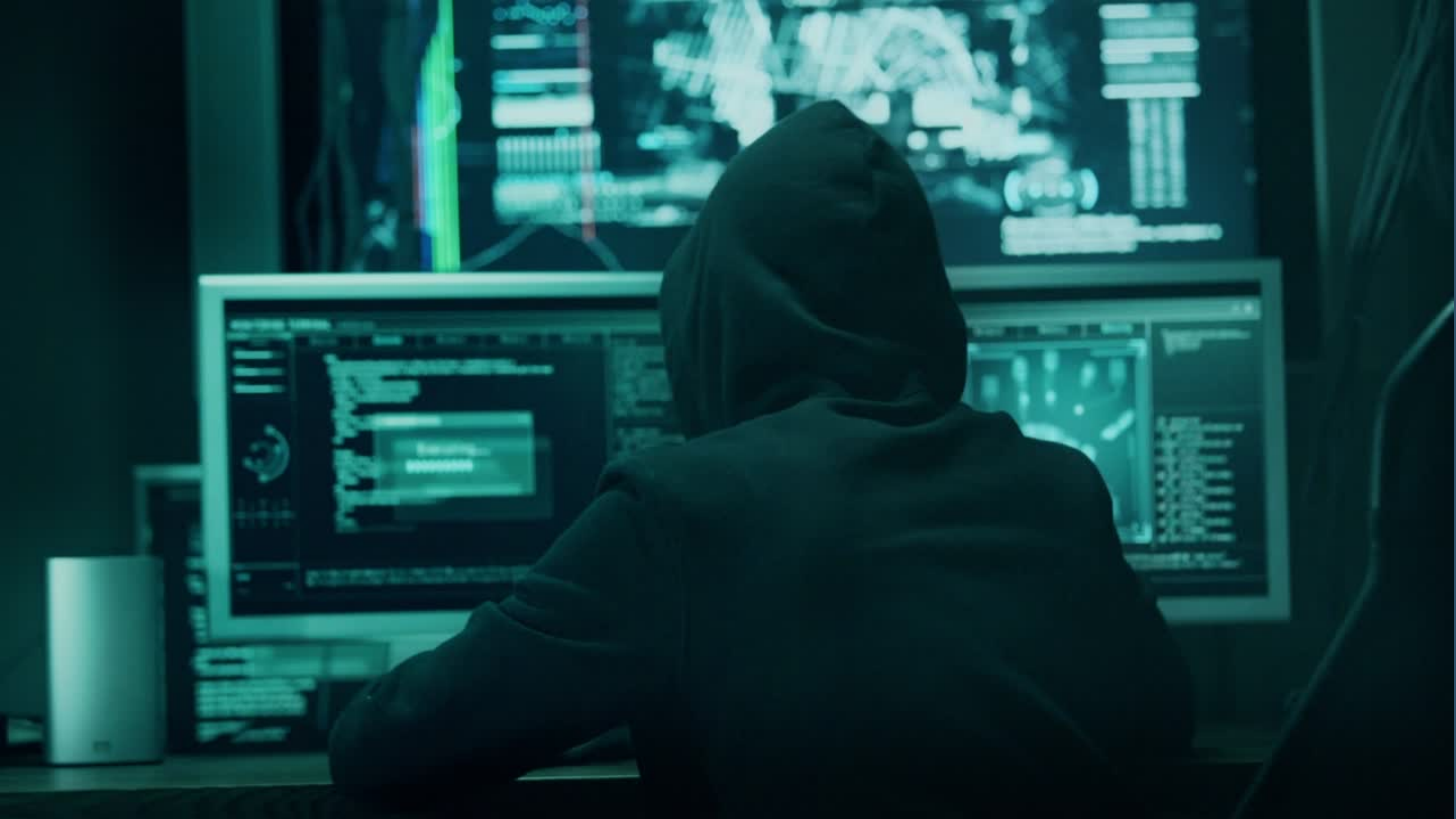


Business as Usual: EI 3.8 Cutoff - 'passenger car production, electric, without battery '- GLO

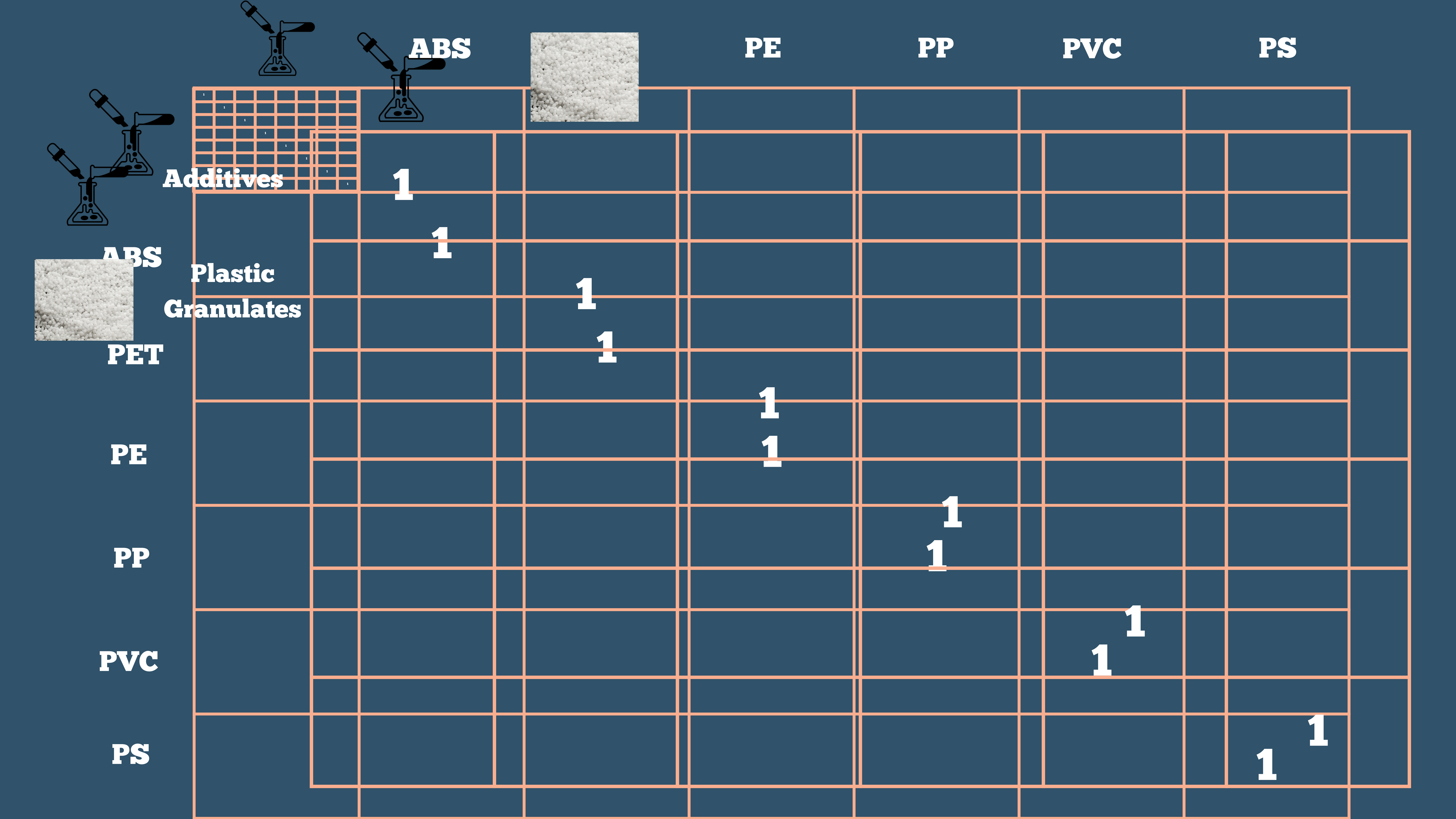


Updated System: EI 3.8 Cutoff - 'passenger car production, electric, without battery - DE

What We Thought Would Happen……



	CaCo3	C(Blk)	Kaolin	C6H4(CO)2O	TiO2	C8H6O4	ZnO	C18H15O4P
CaCo3	1							
C(Blk)		1						
Kaolin			1					
C6H4(CO)2O				1				
TiO2					1			
C8H6O4						1		
ZnO							1	
C18H15O4P								1


ABS
PE
PP
PVC
PS
Additives
Plastic
Granulates
ABS
PET
PE
PP
PVC
PS
1
1
1
1
1
1
1
1
1
1
1
1

Additives	1					
Plastic Granulates		1				
Monomers			1			
PVC-orig.				1		
Car-orig					1	
Elec.-orig.						1

STOCHASTIC ARITHMETIC DISTRIBUTIONS REGIONALIZATION & DEPENDENCIES

				03 PVC					
Additives	1						-[x]		
Plastic Granulates		1			-d; -e		-1	+d; +e	
Monomers		-a; -b	1				+[Δb]		
PVC-orig.		-c		1			+c		
Car-orig					1				
Elec.-orig.						1		+Σ(x)	
Gran.-modif.							1	-d; -e	
Car-modif.								1	
Elec.-modif.								-Σ(x)	1

Results:

Regionalization :

Per 1 kwh

Electric car : medium voltage, GLO

Germany’s (DE) energy mix in

ecoinvent

2022

estimation

2030 educated guess

	Global electricity prod.	DE elec. prod. ecoinvent	DE Energy production in 2022	DE Energy production in 2030 (test scenario)	DE Energy production in 2030 (coal FTW scenario)
(EF v3.0, acidification, accumulated exceedance (ae))	3.48E-03	1.24E-03	1.02E-03	7.74E-04	9.34E-04
(EF v3.0, climate change, global warming potential (GWP100))	**7.07E-01**	**5.64E-01**	**4.66E-01**	**2.31E-01**	**3.31E-01**
(EF v3.0, climate change: biogenic, global warming potential (GWP100))	1.76E-03	7.72E-03	1.02E-02	1.29E-02	1.29E-02
(EF v3.0, climate change: fossil, global warming potential (GWP100))	7.04E-01	5.55E-01	4.55E-01	2.16E-01	3.16E-01
(EF v3.0, climate change: land use and land use change, global warming potential (GWP100))	1.29E-03	7.54E-04	1.22E-03	1.66E-03	1.66E-03
(EF v3.0, ecotoxicity: freshwater, comparative toxic unit for ecosystems (CTUe))	1.30E+01	4.96E+00	3.66E+00	3.33E+00	3.53E+00
(EF v3.0, ecotoxicity: freshwater, inorganics, comparative toxic unit for ecosystems (CTUe))	1.21E+00	3.95E-01	3.42E-01	3.74E-01	3.75E-01
(EF v3.0, ecotoxicity: freshwater, metals, comparative toxic unit for ecosystems (CTUe))	1.18E+01	4.55E+00	3.31E+00	2.94E+00	3.14E+00
(EF v3.0, ecotoxicity: freshwater, organics, comparative toxic unit for ecosystems (CTUe))	3.73E-02	1.50E-02	1.35E-02	1.63E-02	1.56E-02
(EF v3.0, energy resources: non-renewable, abiotic depletion potential (ADP): fossil fuels)	9.18E+00	7.88E+00	5.80E+00	2.53E+00	3.37E+00
(EF v3.0, eutrophication: freshwater, fraction of nutrients reaching freshwater end compartment (P))	3.30E-04	8.40E-04	6.26E-04	1.99E-04	4.90E-04
(EF v3.0, eutrophication: marine, fraction of nutrients reaching marine end compartment (N))	6.66E-04	4.02E-04	3.08E-04	1.63E-04	2.49E-04
(EF v3.0, eutrophication: terrestrial, accumulated exceedance (AE))	6.64E-03	2.81E-03	2.31E-03	1.73E-03	2.03E-03
(EF v3.0, human toxicity: carcinogenic, comparative toxic unit for human (CTUh))	1.63E-10	1.26E-10	1.03E-10	1.16E-10	1.24E-10
(EF v3.0, human toxicity: carcinogenic, inorganics, comparative toxic unit for human (CTUh))	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
(EF v3.0, human toxicity: carcinogenic, metals, comparative toxic unit for human (CTUh))	1.20E-10	9.77E-11	7.84E-11	7.74E-11	8.67E-11
(EF v3.0, human toxicity: carcinogenic, organics, comparative toxic unit for human (CTUh))	4.34E-11	2.87E-11	2.49E-11	3.82E-11	3.76E-11
(EF v3.0, human toxicity: non-carcinogenic, comparative toxic unit for human (CTUh))	6.45E-09	4.92E-09	3.99E-09	3.76E-09	4.37E-09
(EF v3.0, human toxicity: non-carcinogenic, inorganics, comparative toxic unit for human (CTUh))	5.63E-10	6.74E-10	7.46E-10	9.25E-10	9.46E-10
(EF v3.0, human toxicity: non-carcinogenic, metals, comparative toxic unit for human (CTUh))	5.85E-09	4.20E-09	3.20E-09	2.77E-09	3.36E-09
(EF v3.0, human toxicity: non-carcinogenic, organics, comparative toxic unit for human (CTUh))	1.26E-10	7.31E-11	6.52E-11	8.44E-11	8.29E-11
(EF v3.0, ionising radiation: human health, human exposure efficiency relative to u235)	1.04E-01	1.05E-01	3.69E-02	4.95E-03	5.53E-03
(EF v3.0, land use, soil quality index)	**1.35E+00**	**1.05E+00**	**2.02E+00**	**6.25E+00**	**6.25E+00**
(EF v3.0, material resources: metals/minerals, abiotic depletion potential (ADP): elements (ultimate reserves))	9.20E-07	1.14E-06	1.03E-06	2.59E-06	2.57E-06
(EF v3.0, ozone depletion, ozone depletion potential (ODP))	2.33E-08	1.38E-08	1.87E-08	1.37E-08	9.83E-09
(EF v3.0, particulate matter formation, impact on human health)	2.64E-08	4.67E-09	4.24E-09	5.51E-09	5.66E-09
(EF v3.0, photochemical ozone formation: human health, tropospheric ozone concentration increase)	1.79E-03	6.96E-04	5.81E-04	4.33E-04	5.00E-04
(EF v3.0, water use, user deprivation potential (deprivation-weighted water consumption))	1.79E-01	9.28E-02	9.66E-02	1.17E-01	1.27E-01

Plastic Data Improvement :

Per 1 kg

```python
indices = np.array(
    [
        (car_modif, car_modif), # Production exchange for new car
        (passenger_car_prod.id, car_modif)  # the modified car needs the originalcar
    ] + [(id_mod_gran,id_mod_gran) for id_mod_gran in list_id_modified_granulates # Production exchanges for the new granulates
    ] + [(id_ori_gran,id_mod_gran) for id_ori_gran,id_mod_gran in zip(list_original_granulates,list_id_modified_granulates)  # The modified granulates have inpu
    ] + [(inp[0], inp[1]) for inp in inputs_chemicals_to_mod_gran  # The modified granulates have some additional exchanges from chemicals
    ] + [(id_mod_gran, passenger_car_prod.id) for id_mod_gran in  list_id_modified_granulates  #the new car needs the new granulates
    ] + [(id_ori_gran, passenger_car_prod.id) for id_ori_gran in  list_original_granulates   # the new car "produces" the old granulates
    ] + [(id_flow[0],id_flow[1]) for id_flow in inputs_chemicals_to_delete_in_ori_gran  # The new granulates "produce" the replaced inputs
    ] + indices_delta_mass_inputs
    , dtype=bwp.INDICES_DTYPE
)
data = np.array([
        [1 for s in range(size_sample)],  # Production exchange for new car
        [1 for s in range(size_sample)]   # the modified car needs the originalcar
    ] + [ [1 for s in range(size_sample)] for i in range(len(list_id_modified_granulates)) # Production exchanges for the new granulates
    ] + [ [1 for s in range(size_sample)] for i in range(len(list_id_modified_granulates)) # The modified granulates have inputs of original granulates

         #   inp[2] is a list of sampled possible values fot the input
    ] + [inp[2] for inp in inputs_chemicals_to_mod_gran  # The modified granulates have some additional inputs from chemicals

    ] + [[inp_ori for s in range(size_sample)] for inp_ori in inputs_original_granulates_to_car # the new car needs the new granulates

    ] + [[inp_ori for s in range(size_sample)] for inp_ori in inputs_original_granulates_to_car # the new car "produces" the old granulates
    ]  +[[id_flow[2] for s in range(size_sample)] for id_flow in inputs_chemicals_to_delete_in_ori_gran # The new granulates "produce" the replaced inputs
    ] + data_delta_mass_inputs)
flip = np.array(
    [False, # Production exchange for new car
     True   # the modified car needs the originalcar
    ] + [False for i in range(len(list_id_modified_granulates)) # Production exchanges for the new granulates
    ] +[True for i in range(len(list_id_modified_granulates)) # The modified granulates have inputs of original granulates
    ] + [True for i in range(len(inputs_chemicals_to_mod_gran)) #  The modified granulates have some additional inputs from chemicals
    ] + [True for i in range(len(inputs_original_granulates_to_car))# the new car needs the new granulates
    ] + [False for i in range(len(inputs_original_granulates_to_car)) # the new car "produces" the old granulates
    ] + [False for i in range(len(inputs_chemicals_to_delete_in_ori_gran)) # The new granulates "produce" the replaced inputs
    ] +  flips_delta_mass_inputs
```

Launcher | modification car plastics.ipyn | +

Markdown | Python [conda env:bw25]

```
File /opt/tljh/user/envs/bw25/lib/python3.10/site-packages/bw2calc/lca.py:354, in LCA.lci(self, demand, factorize)
    339 """
    340 Calculate a life cycle inventory.
    341 
   (...)
    351 
    352 """
    353 if not hasattr(self, "technosphere_matrix"):
--> 354     self.load_lci_data()
    355 if demand is not None:
    356     self.__check_demand(demand)

File /opt/tljh/user/envs/bw25/lib/python3.10/site-packages/bw2calc/lca.py:206, in LCA.load_lci_data(self, nonsquare_ok)
    200 self.dicts.activity = partial(self.technosphere_mm.col_mapper.to_dict)
    202 if (
    203     len(self.technosphere_mm.row_mapper) != len(self.technosphere_mm.col_mapper)
    204     and not nonsquare_ok
    205 ):
--> 206     raise NonsquareTechnosphere(
    207         (
    208             "Technosphere matrix is not square: {} activities (columns) and {} products (rows). "
    209             "Use LeastSquaresLCA to solve this system, or fix the input "
    210             "data"
    211         ).format(
    212             len(self.technosphere_mm.col_mapper),
    213             len(self.technosphere_mm.row_mapper),
    214         )
    215     )
    217 self.biosphere_mm = mu.MappedMatrix(
    218     packages=self.packages,
    219     matrix="biosphere_matrix",
   (...)
    224     empty_ok=True,
    225 )
    226 self.biosphere_matrix = self.biosphere_mm.matrix

NonsquareTechnosphere: Technosphere matrix is not square: 19574 activities (columns) and 19575 products (rows). Use LeastSquaresLCA to solve this system, or fix the input data
```

Take Aways:

Feedback: