Techno-economic model of CO_2 mineralisation processes for the cement industry Version 1.0

This MATLAB model has been developed for the publication “Towards a business case for CO2 mineralisation in the cement industry” currently under review at Nature communications earth and environment. Here you will find all descriptions of the underlying processes and methods.

When using the entire model or parts cite it as follows: *“Till Strunge, Phil Renforth, Mijndert Van der Spek et al. Towards a business case for CO2 mineralisation in the cement industry, 17 June 2021, PREPRINT (Version 1) available at Research Square [https://doi.org/10.21203/rs.3.rs-478558/v1].”*

The following quick guide will help teach you how to use the provided MATLAB code.

Short general model description

The model is generally designed, that the capacity in how much cement replacement is produced using CO2 mineralisation. The functional unit is t_{SCM} (tonne of supplementary cementitious material produced). The main input is therefore the set capacity or for most model iterations a range of capacities together with process assumptions derived from literature, for example temperature, pressure, yield etc. This is shown in Figure 1.

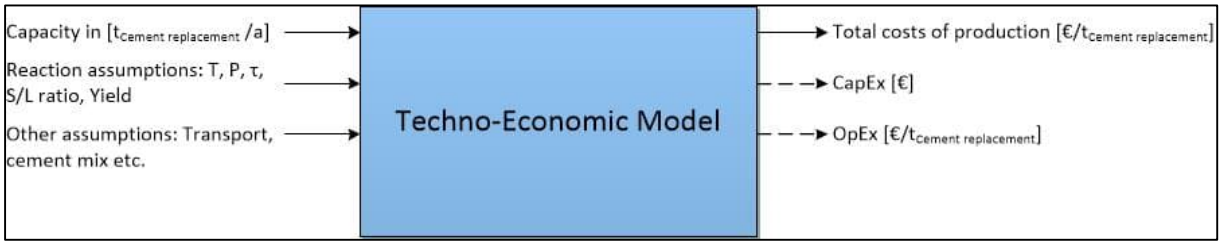

Figure 1: Input / Outputs of the Techno-Economic model.

The model itself is set up so that it can easily be used to test out different assumptions. All calculations are (whenever necessary) based on an input matrix and output matrix, allowing to quickly switch between changes in input parameters, such as mineral composition. This can be shown as follows:

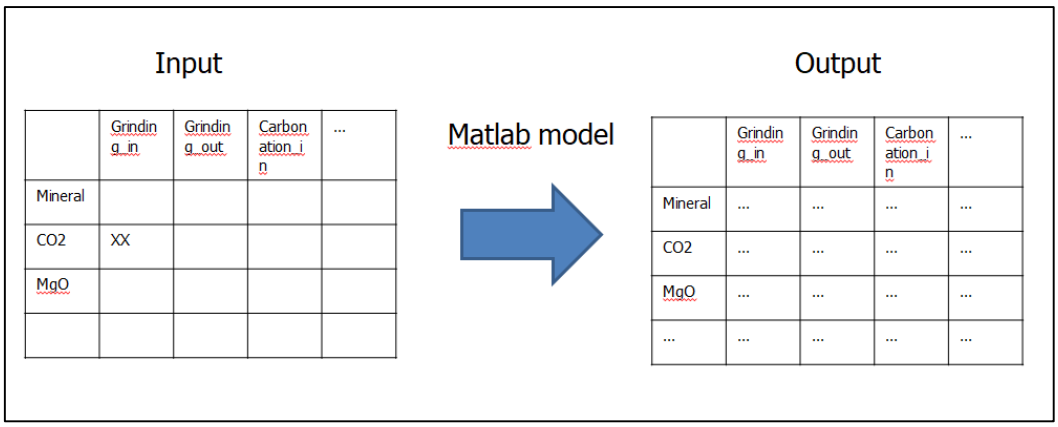

Figure 2: Model - matrix structure

How to get started?

To use the techno-economic model you can either use the scripts for the in the article provided analyses (i.e., MATLAB scripts are provided in the folder 'analyses') or you can use each model (direct and indirect) as functions.

Folder structure

The folder structure of the is shown below. When running the script, these folders should be visible or added to the path, so the Script can find its underlying functions / folders.

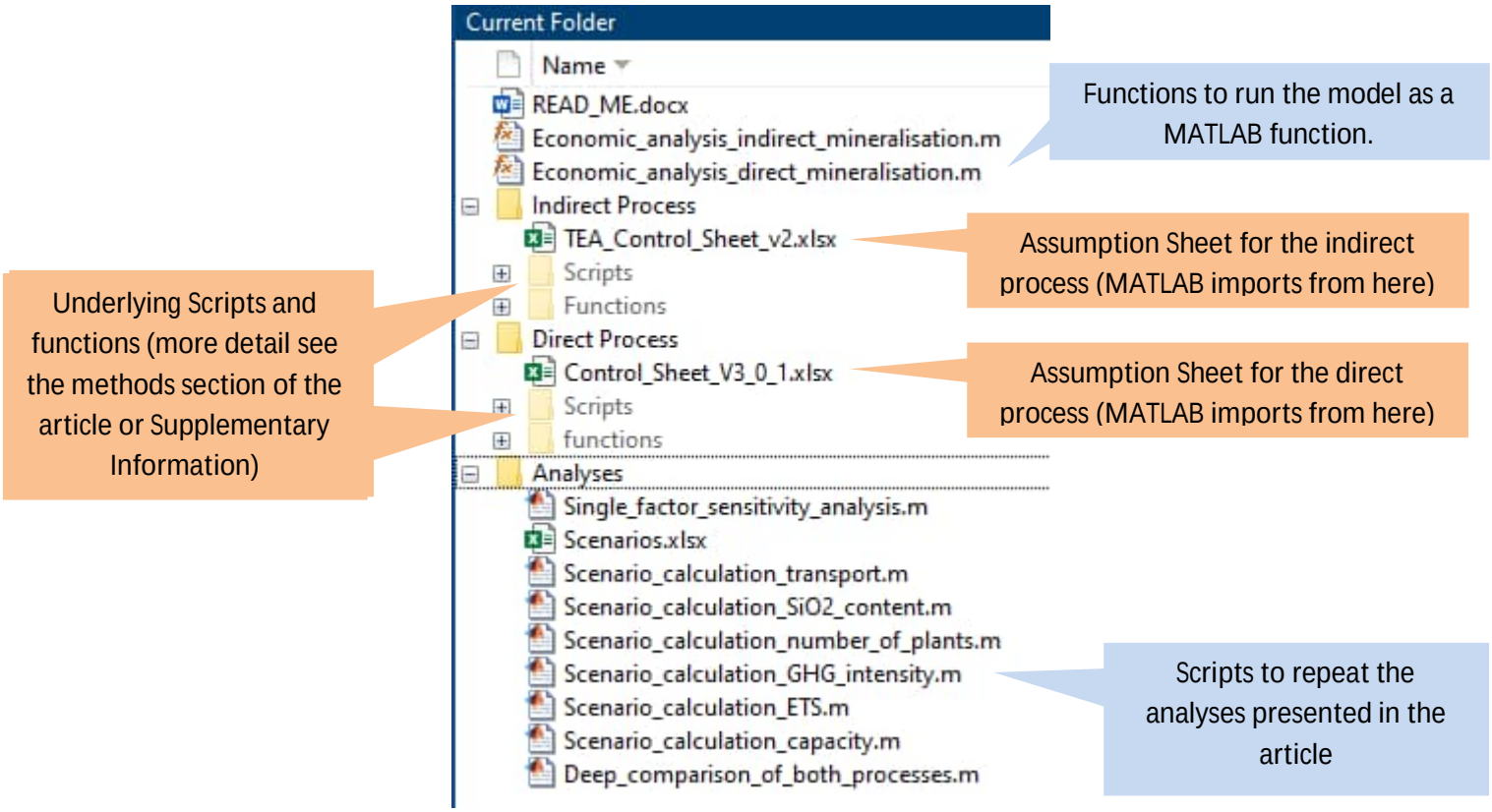

Figure 3: Folder structure and explanation.

Run the script as a MATLAB function

To call the techno economic model as MATLAB functions the input and outputs are as follows. Please note that, the not all inputs have to be given so that the function works in case an input has not been assigned the default value is assumed.

Order of function Inputs: (Number of model runs, Capacity [t_{SCM}/a], Price ETS [€/t_{CO2}], Price Cement[€/t], Share of Silica in cement blend [fraction], Share of inert product in cement blend [fraction], transport distance [km], GHG_intensity_electricity[kg_{CO2eq}/MWh], GHG_intensity_NG [kg_{CO2eq}/MWh])

Order of Outputs:[Levelised_costs_of_product [€/t_{SCM}], Revenue [€/t_{SCM}], Profit [€/t_{SCM}], CO_{2e} emission_reduction [fraction], CO_{2e} emission total [kg_{CO2e}/a]]

An example on how to call this model as a function is shown below.

```
>> [Result_Levelised_costs_of_product,Result_Revenue]= Economic_analysis_direct_mineralisation(3,[100000 10000 250000])

Result_Levelised_costs_of_product =

  146.6253
  261.1823
  130.6168


Result_Revenue =

  135.9320
  135.8162
  135.6720
```

Figure 4: Example of how to call script as a MATLAB function.

Run the predefined Analyses

The Analyses described in the paper "Towards a business case for CO2 mineralisation in the cement industry" are added as separate MATLAB scripts and can be run as well. An overview of each analysis is shown below:

File name	Analysis description
Deep_comparison_of_both_processes.m	Calculation of both processes (indirect and direct) for the mid scenario, exploring capital costs distribution, levelised costs of product (LCOP) distributions etc..
Scenario_calculation_capacity.m	Calculating LCOP and revenue for all 3 scenarios while changing the capacity.
Scenario_calculation_ETS.m	Calculating LCOP and revenue for all 3 scenarios while changing the ETS price.
Scenario_calculation_GHG_intensity.m	Calculating CO2e emission reductions for all 3 scenarios while changing the capacity.
Scenario_calculation_number_of_plants.m	Calculating LCOP and revenue for all 3 scenarios while changing the number of plants built.
Scenario_calculation_SiO2_content.m	Calculating LCOP and revenue for all 3 scenarios while changing the silica content in SCM.
Scenario_calculation_transport.m	Calculating LCOP and revenue for all 3 scenarios while changing the transport distance.
Single_factor_sensitivity_analysis.m	One at a time sensitivity analysis for the mid scenario.

Environmental Assessment

To perform the environmental assessment not all assumptions are supplied in the assumptions excel sheet as some may be proprietary. Hence, the emission factors other than for energy need to be added in the assumption sheets (*Control_Sheet_V3_0_0_1.xlsx* for the direct process and *TEA_Control_Sheet_v2.xlsx* for the indirect process respectively). This is shown in the following figures. Missing values are marked in red.

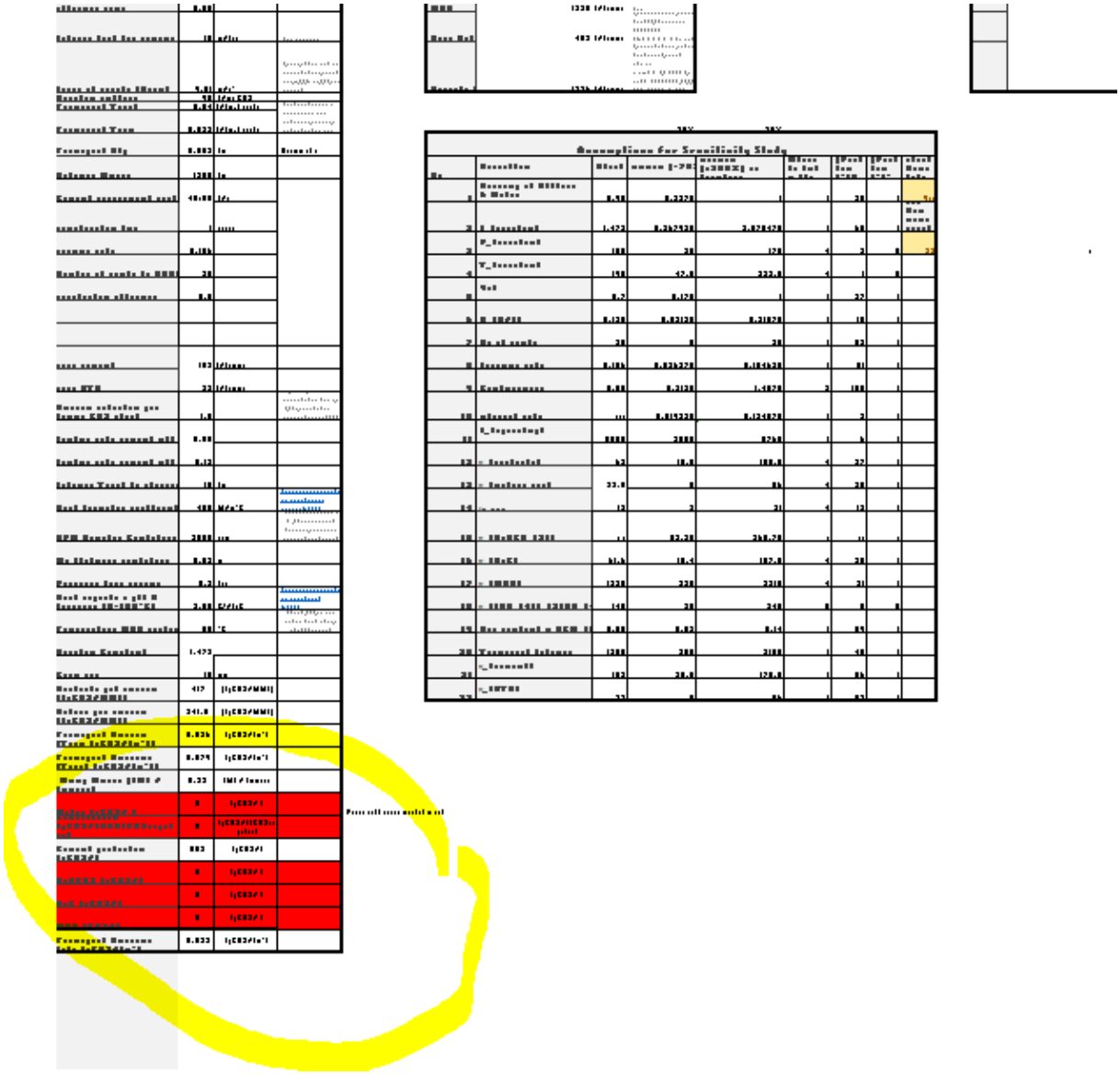

Figure 5: Exerpt from the Control sheet.