biODYM quick-start guide

Part I Qualitative model

0 Load packages

ODYM framework
- ODYM_classes
- ODYM_functions
- dynamic_stock_model

Packages (ODYM)
- sys, os
- numpy
- pandas
- matplotlib.pyplot
- pickle
- pylab

Packages (biODYM)
- plotly.graph_objects
- ipywidgets
- xlsxwriter
- scipy.stats

Notes

- Load ODYM via local path.

- Install packages via pip terminal and load via "import" in notebook.

1 Definition of system and relevant aspects

System aspect Time
- Dimension = Time (t)
- Items = MyYears

System aspect Element
- Dimension = Element (e)
- Items = Good, Carbon

IndexTable

Define Processes (P)
- Name
- ID

ProcessList

Define Flows (F)
- P_Start & P_End
- Indices

FlowDict

Define Stocks (S)
- P_Res
- Type
- Indices

StockDict

ODYM data base

Notes

- Model initiating routines are very rigid, so no need to change a lot. If more Elements (e.g. Nitrogen) or more years should be considered, they can be easily added.

- System components (P, F, S) have no values yet but empty arrays.

- ODYM data base is the model foundation. The further procedures always refer to it.

Part II Quantitative model

2 Data input into model

biODYM input_data_template.xlsx

Parameters
- Importflows
- Transfer coefficients (TC)
- Uncertainty

ParameterDict

Consistency_Check()
- Dimension consistency
- Process index consistency
- Flow value array consistency

ODYM data base

Notes

- All input data gets stored as parameters.

- Consistency_check() is an ODYM-inherent function that allows to confirm general system definition consistency.

3 MFA Calculations

MFA solution (w/o FOMP)
- Importflows from ParameterDict
- Other F and S by TC calculations independent of FOMP

FOMP

Manual data input

BioParameters
- Values
- Uncertainty
- P_Res

BioParameterDict

FOMP calculations

MFA solution (w/ FOMP)
- Remaining F and S by TC calculations

ODYM data base

MassBalance()
- Balance dimensions (time steps x process x element)
- Balancing errors

Notes

- FOMP = First order model process

- Qualitative data is combined with quantitative data to calculate results.

- FOMP procedure is separated from ODYM procedure. After calculations, FOMP results are then used to calculate remaining non-FOMP F and S and all results are finally stored in the ODYM data base.

- MassBalance() is an ODYM function that checks if mass balance principle is fulfilled.

extract

Monte-Carlo-Simulation (MCS)

Manual data input

MCS Parameters
- Model runs = 10.000
- Probability density function = log-norm.

BioParameterDict

ParameterDict

Generate pseudo-random values

MC_BioParameterDict

MC_ParameterDict

MCS

Repeat previous calculations with MC dictionaries

MC_FlowDict

MC_FlowDict_absSTD

MC_StockDict

MC_StockDict_absSTD

Notes

- MCS in essence repeats calculations, but with 10.000 values per parameter according to log-norm. probability density

- MCS results are stored separated from ODYM data base

- absSTD = Absolute standard deviation

Part III Conclude MFA

4 Presentation of results

Static Results presentation
- System results simple plots
- MCS simple plots and violin plots

MC_FlowDict

MC_FlowDict_absSTD

MC_StockDict

MC_StockDict_absSTD

ODYM data base

Sankey diagram data
- Processes
- Flows
- Colours

Interactive Sankey diagram
- sankey_diagram_results()

Excel export
- System results
- MCS results

Notes

- System results can be displayed as static simple plots or interactive Sankey diagram.

- For interactive Sankey diagrams, relevant data is converted into applicable form from ODYM data base.

- MCS results can be displayed as simple plots or violin plots.

- All results can be exported to Excel.

Legend

ODYM

Storage

biODYM extension

Activity
- Most important items

Data definition
- Most important items

Data input