ECO2DES: Python Framework for the Eco-Design of Industrial Processes

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Abstract

More than 80% of the costs and environmental impacts of a new process are defined in the design phase, often without being properly assessed. ECO2DES is a new methodological approach for the eco-design of industrial processes (chemical, petrochemical, energetic, bio-based…), integrated in a Python framework. ECO2DES allows for maximising economic parameters such as the net present value, and minimising environmental impacts by the integration and automation of modelling, process simulation, life cycle assessment (LCA), life cycle costing assessment (LCC) and multi-objective optimisation algorithms (MOOA). This new methodology does not only design the optimal process from and sustainable point of view, but also reduces the workload accelerating the time-to-market of research and innovative projects in the process industry. In order to illustrate the potential of the framework, the methanation process for energy storage will be evaluated. The outputs of the ECO2DES framework clearly mark the way for the detailed engineering in the development of this process.

Keywords: Eco-design, process simulation, life cycle assessment, life cycle costing, optimisation.

1. Introduction

During the development of new innovative processes, there are no industrial data that can support any life cycle assessment, LCA, or life cycle cost, LCC, study, which gives rise to numerous trial-and-error phases during technology upscaling, exorbitantly increasing time-to-market and costs. Predictive models and process simulations, however, are able to compute, through physicochemical relationships, the behaviour of that technology under development at industrial scale and formulate scenarios for environmental or cost optimisation. However, process simulation, LCA and LCC methodologies are well structured and there are many options of commercial software specialised in these areas. Nowadays, at the best of our knowledge, there is no current research combining them in a holistic way for their application in the economic and environmental optimisation of any industrial design of process under research and/or development. With this premise, the ECO2DES framework was born. It is an object-oriented Python framework for sustainability-oriented optimisation of industrial processes. The tool takes advantage of the full feature set of Python, such as its facilities for fast prototyping and the several available libraries for data processing, data analysis, scientific computing and data visualisation. ECO2DES is a descriptive tool, which documents life cycle inventories and characterises them through their environmental impact and associated costs. It is a
predictive tool, since it uses as inputs physicochemical models for process simulation in the research phase; and adaptive, since it automates process design selections based on multi-objective optimisation algorithms.

2. ECO2DES architecture

The architecture scheme of ECO2DES is illustrated in Fig. 1. It has an object-oriented design to make it flexible and expandable.

![Figure 1. ECO2DES architecture scheme.](image)

The core classes of ECO2DES are projects, simulation, lca, lcc and optimization. Class projects encapsulates the management tools, it offers several methods to create, delete, copy and assign projects. The initialisation of ECO2DES framework creates a folder inside the home directory in which all the projects are stored. Every project is linked to its own Ecoinvent 3.6 databases (Wernet et al., 2016), in order not to interfere with the changes made in another project. Class simulation allows to link with a model or simulation developed in Python, Excel or Aspen Plus, as well as defining the inputs and outputs of the simulation. Class lca inherits the most of its methods from Brightway2, (Mutel, 2017) an open-source framework for life cycle assessment. Some improvements regarding speedup calculation inside an optimisation loop, as well as several data visualisation tools were aggregated. Furthermore, this class allows the user to link the inputs and outputs defined in the class simulation with exchanges of an existing activity inside the database or a new one previously created. Class lcc was developed from scratch. It solves a financial life cycle costing of the product or products (from cradle to customer), but further implementations will be made to include a whole life cycle evaluation (from cradle to gate) and compute externalities costs derived from the environmental impacts assessed in the class lca. Finally, class optimization has methods to define the problem with variables from the classes simulation, lca and/or lcc; their boundaries, the problem constrains and the objectives from the three abovementioned classes. Class optimization has several algorithms for heuristic global optimisation and local optimisation, with a single or multiple objectives. These algorithms are inherited from pygmo (Biscani et al., 2010) and scipy (Virtanen et al., 2019), other libraries are under study to include their features, as well as own-developed implementations.
3. Case study: Sabatier for renewable energy storage in the natural gas grid

3.1. Background

Currently, conventional energy sources such as nuclear power or fossil fuels are being replaced by renewable ones such as wind or solar energy. However, most of the renewable sources cannot provide a base load electric power. To overcome this problem, storage systems have to be integrated in the power grid. For seasonal storage of the energy (charge / discharge period from 1 day to 1 year) in huge capacities, electrical energy can be converted into chemical energy by transferring it into fuels. The logical pathway is the conversion of electrical energy into hydrogen by water electrolysis, but nowadays there is no a hydrogen grid or a large enough storage system developed in any country. Until this requirement is satisfied, the highly developed natural gas grids can be used for the transport of excess energy (Bassano et al., 2019), using electrolysis to produce hydrogen to react with carbon dioxide in a methanation synthesis. So in addition to providing an energy carrier, the process consumes carbon dioxide, contributing to the reduction of GHGE. The methanation reactions of carbon monoxide and carbon dioxide were discovered at the beginning of the 20th century by Sabatier et al. (1902). The methanation of carbon dioxide is an exothermic catalytic reaction and is typically operated at temperatures between 200°C and 550°C depending on the used catalyst.

3.2. Sabatier process simulation

For the determination of the optimal reactor concept, the kinetic model 12 of Kopyscinski (2010) was used. The model parameters were implemented within a RPLUG reactor of Aspen Plus. Furthermore, the resulted gases are connected to a RGIBSS reactor to minimise the free energy of Gibbs following the Boudouard reaction (Gao et al., 2012). This way the potential formation of coke will be measured and taken into account for the deposition of solid over the catalysts, and, therefore, the economic model would take into account the regeneration and replacement cycles of the catalyst. The heat of the gas stream is recovered in the inlet current of the reactor as well as in the hybridisation with a Rankine cycle to generate electricity, which operates with water or cyclopentane as working fluid. Finally, the gas is dried and compressed to be injected into the grid. Then, if the hydrogen molar composition is higher than a 5 % a pressure swing adsorption, PSA, unit is needed, recovering 90 % of the hydrogen which is recirculated. Moreover, if
carbon dioxide molar composition is higher than a 2 % a monoethanolamine (MEA)-based capture is needed, recovering 97% of the dioxide of carbon which is then recirculated. Both of them modelled as black boxes. Fig. 2 illustrates the layout of the Aspen Plus simulation.

3.3. ECO2DES implementation

3.3.1. Project creation and simulation linking

After importing ECO2DES framework, the first step is setting a project by name (if the project does not exist, this method creates it) and link it to the Aspen Plus simulation:

```python
import eco2des as e2d
e2d.projects.set_current('Sabatier_case_study')
e2d.simulation.link('Sabatier_k.bkp')
aspen = e2d.simulation.com
```

Once the link method of the class simulation is run, the com object of the Aspen Plus simulation is created as an attribute of the class (see line 6 of the above code). This com object could be used to get access to the whole simulation data (for further understanding, please visit the Aspen Plus user guide, ActiveX section (AspenTech, 2010)), and with the define_input and define_output methods the variables of interest could be built.

3.3.2. Life cycle assessment

When the simulation is linked and the inputs and outputs defined, the life cycle assessment of the process could be modelled. The following code illustrates as an example how a database is picked, how a new activity is created and how a technosphere exchange is added to it:

```python
ei36 = e2d.lca.database('Ecoinvent 3.6 cutoff')
sabatier = ei36.create_activity(name = 'Sabatier for storage of renewable energy in the gas grid', location = 'ES', unit = 'cubic meter', ref_product = 'SNG', production_amount = 1.0)
wastewater = [act for act in ei36 if act['name'] == 'market for wastewater, from residence' and act['location'] == 'Row'][0]
sabatier.new_exchange(amount = -1*e2d.outputs['waste water'] / e2d.outputs['SNG'], input=wastewater, type='technosphere').save()
```

3.3.3. Life cycle costing assessment

When the simulation is linked and the inputs and outputs defined, the life cycle costing assessment of the process could be modelled. The following code illustrates as an example how the LCC object is instanced, how the reactor vessel is assigned to an ECO2DES correlation which calculates the cost based on the material needed computed based on the ASME BPVC, section VIII, division 1 (ASME, 1986). Finally, it shows how a William’s correlation is used to compute the PSA cost.

```python
lcc = e2d.lcc(local_factor = 0.89)
lcc.vessel(Q = e2d.outputs['Flow in'], rt = e2d.outputs['Residence time'], p=1e6, LD = e2d.inputs['LD ratio'], T = e2d.inputs['Reactor temperature'], phase = 'Fluids', kind = 'horizontal', material = 'Stainless 304', name = 'Sabatier reactor vessel')
lcc.william_equipment(name = 'PSA', cap = e2d.outputs['H2 recover']*[0.89/1800]*24, n = 0.7, ref_cap = 155.24, ref_cost = 7.32e6, ref_CEPCI = 444.2, phase = 'Fluids')
```

3.3.4. Multi-objective optimisation

Finally, the following code shows how a multi-objective optimisation problem is defined in ECO2DES (line 2), the optimisation algorithm is picked in line 1, in this case the multi-objective evolutionary algorithm with decomposition (MOEA/D) is used. An initial population is randomly constructed in line 12 and evolved in line 13. The problem has some constrains marked, based on the regulations for the natural gas grid: hydrogen composition lower than a molar 5 %, monoxide of carbon and dioxide of carbon composition lower than a molar 2 %. In this case, the constrains are treated as penalties during the simulation outputs definition.
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3.4. Results

The storage efficiency is measured as the lower heating value (LHV) of the SNG divided by the electricity used (wind power for electrolysis minus the generated power). For LCA, the functional unit is 1 Nm$^3$ of SNG without considering the combustion and the limits of the system consider CO2 as free of environmental burdens, since it is a waste from the capture process. In this example, the climate change is assessed following the IPCC 2013 method without long term emissions for the characterization of the global warming potential. The levelised cost is calculated taking into account the capital expenditure (CAPEX) and operational expenditure (OPEX) assuming a loan of 60 % of CAPEX with a period for payment of 10 years and an interest of 4 %. A discount rate of 10 % is used during the 30 years of lifetime and a construction time of 1.5 years is assumed. The Pareto front for the three objectives optimisation problem is shown in Fig. 3. Moreover, two additional optimisation problems were solved using the non-dominated sorting genetic algorithm (NSGA-II): a two objectives problem with the storage efficiency and the levelised cost of SNG (see Fig. 4) and other with the climate change and the levelised cost of SNG which showed that these objectives are non-conflicting. The optimal solution of the methanation process, from the environmental and economic points of view, corresponds to the following conditions: hydrogen to carbon dioxide mole ratio of 4.44, a reactor temperature of 396 °C, a reactor length of 2.64 m, a reactor length to diameter ratio of 5.72 and using water as working fluid in the Rankine cycle. The calculated levelized cost of SNG is 1.481 €/Nm$^3$, the climate change impact is 1.088 kg CO2-eq./Nm$^3$ and the storage efficiency is 57.95 %. With this configuration a hydrogen recovery system is required, but carbon dioxide conversion is 98.63 % which allows injection SNG to the grid without recovering it.
Figure 4. Methanation for energy storage using NSGA-II: Population evolution (left) and Pareto front (right).

4. Conclusions

ECO2DES, a Python-based framework for sustainability-based optimisation of industrial processes, has been presented in this paper. It provides support for accelerating the time-to-market of novel processes in different industries: automating the LCA and LCC, solving multi-objective and single-objective problems and performing upscaling studies. As an example, the methanation process has been analysed inside the framework. The results mark the way for the detailed engineering in the development of this process, showing that, on the one hand, environmental and economic objectives are non-conflicting. On the other hand, to improve storage efficiency will always compromise the environmental and economic performance of the process.

References

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