Design of Life cycle models using Structural Path Analysis under Uncertainty

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Supporting Information

1 Toy Problem

As defined in the main paper, the model generation algorithm starts the the disaggregation of the primary process from the economy model for performing Structural Path Analysis (SPA). The IO model is available in the form of Make and Use matrices, $\overline{\mathbf{V}}$ and $\overline{\mathbf{U}}$. In actual case studies, the IO model would be available to the user. However, for this toy problem, we had to build an IO model to explain the algorithm. IO models are built by averaging huge number of similar processes with significantly different production capacities using monetary information. In this example, we aggregate 20 Processes 1 and 2 and 10 Process 3 systems. The base Process 3 which is aggregated is considered to have an output of 25 kg of F_7.

$$\overline{\mathbf{V}} = \begin{bmatrix} 994.20 & 0 & 0 \\ 0 & 981.95 & 0 \\ 0 & 0 & 375 \end{bmatrix} \tag{1}$$

$$\overline{\mathbf{U}} = \begin{bmatrix} 0 & 389.76 & 302.22 \\ 579.00 & 0 & 201.48 \\ 0 & 0 & 0 \end{bmatrix} \tag{2}$$

Primary Process P_3 is disaggregated by using Eq. 26-35 from Hanes and Bakshi.

$$\overline{\mathbf{V}}^* = \overline{\mathbf{V}} - \hat{\mathbf{p}}\mathbf{P}_P^E\mathbf{V}\mathbf{P}_F^E \tag{3}$$

$$\overline{\mathbf{V}}^* = \begin{bmatrix} 994.20 & 0 & 0 \\ 0 & 981.95 & 0 \\ 0 & 0 & 375 \end{bmatrix} - 1.5 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} [25] \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \tag{4}$$

$$\overline{\mathbf{V}}^* = \begin{bmatrix} 994.20 & 0 & 0 \\ 0 & 981.95 & 0 \\ 0 & 0 & 337.50 \end{bmatrix} \tag{5}$$

$$\overline{\mathbf{U}}^* = \overline{\mathbf{U}} - \mathbf{X}_u^E\mathbf{P}_P^E \tag{6}$$

$$\overline{\mathbf{U}}^* = \begin{bmatrix} 0 & 389.76 & 302.22 \\ 579.00 & 0 & 201.48 \\ 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 30.22 \\ 20.15 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \tag{7}$$

$$\overline{\mathbf{U}}^* = \begin{bmatrix} 0 & 389.76 & 271.99 \\ 579.00 & 0 & 201.48 \\ 0 & 0 & 0 \end{bmatrix} \tag{8}$$

The primary process which was subtracted out from the original IO model is now added as a separate sector to create new make and use matrices.

$$\overline{\mathbf{V}}_n^* = \begin{bmatrix} 994.20 & 0 & 0 & 0 \\ 0 & 981.95 & 0 & 0 \\ 0 & 0 & 337.50 & 37.5 \end{bmatrix} \tag{9}$$

$$\overline{\mathbf{U}}_n^* = \begin{bmatrix} 0 & 389.76 & 271.99 & 30.20 \\ 579 & 0 & 181.33 & 20.15 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{10}$$

Using Eq. **??**, the Direct Requirements matrix is calculated.

$$\overline{\mathbf{A}}_n^* = \begin{bmatrix} 0 & 0.40 & 0.81 & 0.81 \\ 0.58 & 0 & 0.54 & 0.54 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{11}$$

The economy scale environmental interventions matrix is calculated using equipment scale data and price information. $\overline{B} = [0.0164; 0.084; 0.2; 0.2]$. Initialization of model generation algorithm starts with the IO model. The P2P matrix is established as

$$\overline{\underline{X}} = I - \overline{\underline{A}}_n^* = \begin{bmatrix} 1 & -0.40 & -0.81 & -0.81 \\ -0.58 & 1 & -0.54 & -0.54 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{12}$$

Final demand from this model is 15kg of product F˙7 from Process S˙3. As we are working with only an IO model, the final demand is rewritten in monetary terms as

$$\overline{\underline{F}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 22.5 \end{bmatrix} \tag{13}$$

g for this model is calculated as

$$g = \overline{\underline{BX}}^{-1}\overline{\underline{F}} = 7.46 \tag{14}$$

Relative Standard Deviation (RSD) is calculated using

$$RSD = \frac{\sigma(\overline{\underline{BX}}^{-1}\overline{\underline{F}})}{(\overline{\underline{BX}}^{-1}\overline{\underline{F}})} \tag{15}$$

$\sigma(\overline{\underline{BX}}^{-1}\overline{\underline{F}})$ is calculated using Eq. 36 from the main paper. A matlab code is used for performing this calculation which is provided with the supplementary files. For this calculation, we have used toy_model1.m file. Thus RSD is obtained as

$$RSD = \frac{5.77}{7.46} = \mathbf{0.77} \tag{16}$$

For complexity calculations, $Model1$ has four activities all modelled in the economy scale. From the complexity information in Table 3, M_c for this model is calculated as

$$M_c = \overline{np} + \underline{np} + np \tag{17}$$

$$M_c = 4 * 1 = 4 \tag{18}$$

In the next iteration, a new model is generated with lower RSD. From SPA results in Table 2, it is observed Process S3 has the largest contribution to environmental impact. Thus, for the next model, S3 is removed from the economy scale and modelled at the equipment scale using process information directly from the engineering information at the beginning of the Methodology section. That is achieved easily by replacing the last row and column in the previous $\overline{\underline{X}}$ matrix with engineering scale information. 21.01 and 14 in the cut off matrix is obtained by multiplying solution of F3 and F5 from Table 1 for F7 of 15 kg with the corresponding prices.

$$\overline{\underline{X}} = \begin{bmatrix} 1 & -0.40 & -0.81 & -21.01 \\ -0.58 & 1 & -0.54 & -14 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 15 \end{bmatrix} \tag{19}$$

The interventions and final demand vectors is also redefined with physical information as

$$\overline{\underline{B}} = \begin{bmatrix} 0.01640.08410.24.5 \end{bmatrix} \tag{20}$$

$$\overline{\underline{F}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 15 \end{bmatrix} \tag{21}$$

g for this calculated using Eq. 30 as **7.93**. Complexity of the model is calculated using Eq. 17. RSD is again calculated using Eq. 15 with the numerator uncertainty term calculated by using matlab file toy_model2.m.

$$RSD = \frac{5.30}{7.93} = \mathbf{0.66} \tag{22}$$

Two activities are modelled in the economy as one in the equipment scale. Thus M_c is calculated as

$$M_c = 3 * 1 + 1 * 100 = 103. \tag{23}$$

To reduce RSD further, the model is rearranged further. From the SPA results in Table 2 of the main paper, we find that the first order linkages of S_1 and S_2 to S_3 have high contributions to the environmental impact. So both these linkages are now modelled in the value chain scale. For this, one process S_1 and one process S_2 are disaggregated using Eq. 3 and 6 from the economy scale and remodelled in the value chain scale. New make and use matrices are obtained as

$$\overline{\mathbf{V}}_n^* = \begin{bmatrix} 944.49 & 0 & 0 \\ 0 & 932.85 & 0 \\ 0 & 0 & 337.50 \end{bmatrix} \tag{24}$$

$$\overline{\mathbf{U}}^* = \begin{bmatrix} 0 & 370.27 & 271.99 \\ 550.05 & 0 & 181.33 \\ 0 & 0 & 0 \end{bmatrix} \tag{25}$$

The new P2P multiscale matrix is obtained as

$$\underline{\overline{X}} = \begin{bmatrix} 1 & -0.40 & -0.81 & 0 & -13.40 & 0 \\ -0.58 & 1 & -0.54 & -24.51 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 13 & 0 & -7 \\ 0 & 0 & 0 & 0 & 16.64 & -5.6 \\ 0 & 0 & 0 & 0 & 0 & 15 \end{bmatrix} \tag{26}$$

In actual problems, the life cycle inventory will be obtained from databases. However, in our example, we have to create such a database that mimics the nature of actual life cycle inventories. For that purpose, we averaged up two systems, one producing 25 kg of F7 and another producing 15 kg. These calculations are not pertinent to the algorithm functioning and are not described in details. It was using these values that columns 4 and 5 were filled. Similarly the interventions matrix is also built using life cycle inventory information.

$$\underline{\overline{B}} = \begin{bmatrix} 0.02 & 0.08 & 0.20 & 0.71 & 3.49 & 4.50 \end{bmatrix} \tag{27}$$

Finally F is defined for the new model as

$$\underline{\overline{F}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 15 \end{bmatrix} \tag{28}$$

Finally using Eq. 17, we find g = 7.99. Using Eq. 15 and toy_model3.m file for uncertainty calculation, RSD is calculated.

$$RSD = \frac{3.03}{7.99} = \mathbf{0.38} \tag{29}$$

$Model3$ has three activities modeled at economy scale, two at value chain and one at equipment with brings total M_c to 123. This is the best possible model we can get as the upper limit on M_c does not allow any other shifts from value chain to equipment.

2 Biodiesel Case Study

For the biodiesel case study, a 2007 US IO model is used as the economy scale for SPA calculations and model generation. As mentioned in main paper, disaggregation was not necessary and SPA is done directly on the 380 sector IO model with biodiesel added separately as the 380th sector. The information for building this sector is obtained from the engineering process model and converted in to dollar units using price information. Using the new make and use matrix, new 380 sector $\overline{A}$ matrix is obtained to build the new P2P $\underline{\overline{X}}$ matrix as shown in Eq. 11 and Eq. 12 in the toy problem supporting information. The make $\overline{U}$, use $\overline{V}$ and $\underline{\overline{X}}$ matrices are provided in the SPA.mat file.

After obtaining the SPA results as seen in Table 4 of the main paper, the model generation algorithm starts. The initial model as mentioned in Methodology is the US IO model. The matlab files with the loaded matrices, excel data files are provided in the Step1.zip folder. Using the 380 sector model built previously, g is calculated as

$$g = \overline{\underline{BX}}^{-1}\overline{\underline{F}} = 0.36 \tag{30}$$

Uncertainty data of the model is loaded in the Step1.mat file. Using the *uncertainty* script, the RSD of the model is calculated to be

$$RSD = \frac{5.94}{0.36} = \mathbf{16.50} \tag{31}$$

Granularity based complexity parameter is used for this case study. The data is provided with the granularity.csv file. For the initial model, the granularity is calculated as sum of the granularity information of the individual sectors in the economy model.

$$M_c = \overline{na}^{-1} = \sum_k a_k^{-1} \tag{32}$$

where k is the number of sectors in IO model. Using data provided in the economy sheet in the granularity.csv file, M_c is calculated to be

$$M_c = 1.23 \tag{33}$$

This value is obtained by summing up the numbers in the column marked granularity inverse. As the M˙c is still within the limit, RSD can be reduced further. Going back to the SPA results in Table 4 from the main paper, it is observed that the activity of 22 (Electric generation) supplying products to 248 (Basic Inorganic chemical manufacturing) and then from 248 to 380 (biodiesel manufacturing sector) needs to be modelled at a higher quality scale. Thus as demonstrated in the Toy example, using Eq. 3 and Eq. 4, the respective sectors are disaggregated from the economy model using information and then remodelled as value chain scale activities, using information from the life cycle inventory databases. The P2P $\overline{\underline{X}}$ matrix is rebuilt and is supplied in the Step2.mat file as well as in the Step2.xlsx file.

Uncertainty data of the model is loaded in the Step2.mat file. Using the *uncertainty* script, the RSD of the model is calculated to be

$$RSD = \frac{14.28}{5.46} = \mathbf{2.62} \tag{34}$$

Using data provided in the economy sheet as well as the value chain sheet in the granularity.csv file, M_c is calculated to be

$$M_c = 1.23 + 0.00295 + 0.5 \tag{35}$$

These steps are iteratively repeated until we reach the final model as shown in Fig. 10b of the final paper. In the final step, the biodiesel activity is moved to the equipment scale for reasons mentioned in the main text. The different steps (models built iteratively) are provided in respective .mat files, with data in the .xlsx files. The uncertainty scripts for calculating RSD are also provided for the individual steps.