Multi-scale Sustainable Engineering: Integrated Design of Reaction Networks, Life Cycles, and Economic Sectors

Vyom Thakker and Bhavik R. Bakshi*

William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, Ohio 43210, The United States

Appendix

This appendix contains a tutorial for explaining the computation of sub-matrices of the multi-scale matrix, shown in Equation 7. This equation has been duplicated in the appendix for continuity, as shown below.

$$\begin{bmatrix} \overline{I}-\overline{A}^*(\{\underline{s},s^r\}) & -\underline{X}_u & -X_u^E \\ -\underline{X}_d & \underline{A}^*(\{\underline{s},s^r\}) & -X_u^V \\ -X_d^E & -X_d^V & A' \end{bmatrix} \begin{bmatrix} \overline{s} \\ \underline{s} \\ s^r \end{bmatrix} = \begin{bmatrix} \overline{f} \\ \underline{f} \\ f^r \end{bmatrix} \tag{A.1}$$

This tutorial relies on the illustrative example described in section 3.2 . The superstructure network for this example is redrawn in figure A.1, from figure 4 (a) . The number of economy sectors, value-chain processes and reactions in the illustrative example are each two. The inter- and intra- scale flows are found using the matrices and parameters listed in Equation 20 . Following sections will demonstrate how we compute various elements of the multi-scale matrix, starting from the finest scale, namely reaction scale.

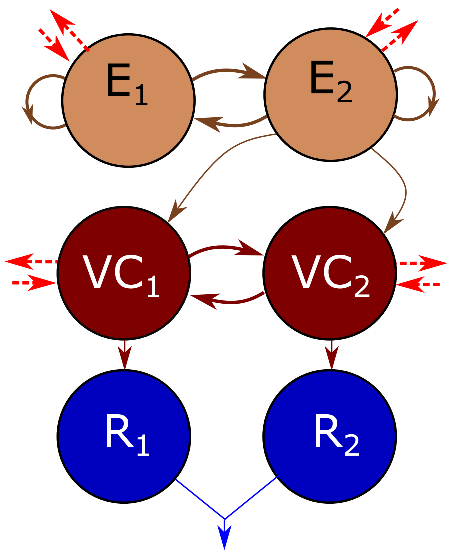

Figure A.1: Illustrative Example, Superstructure Network assuming no need for disaggregation

*Corresponding Author: B.R. Bakshi (bakshi.2@osu.edu)

A.1 Reaction Scale

The reaction scale is represened by the stoichiometric matrix A^r, similar to the Reaction Network Flux Analysis (RNFA) model. However, to use the P2P-RNFA framework with disaggregation of chemical reactions from coarser scales, disaggregation is needed. As evident from section 3.1.2, disaggregation operation is performed on the make and use matrices. Therefore, it might be neccessary to decompose the stoichiometric matrix A^r into make and use matrices (V^r and U^r) . This is done by considering only reactants (negative coefficients) in the use matrix, and products (positive coefficients) in the make matrix, thereby satisfying the relation $A^r = V^{rT} - U^r$.

The interpretation of make and use matrices and their role in the multi-scale network is demonstrated using the illustrative example. As shown in figure A.3, there are two reactions, R_1 and R_2 in the reaction scale, both yielding a single product, which is desirable outside the system. To produce 1 mole of output, R_1 consumes 0.01 kg of raw material (say p_1) coming from the first value-chain activity, i.e. VC_1. Similarly, R_2 consumes 0.02 kg of p_2, coming from VC_2 to produce 2 moles of output. Since, the flows coming from the value-chain scale are not intra-scale flows, they won't be present in the use matrix A^r, but will be present in the upstream cut-off from the value-chain scale, i.e. X_u^V. Therefore, the use matrix is a 0 matrix ($\begin{bmatrix} 0 & 0 \end{bmatrix}$), and the make matrix is $\begin{bmatrix} 1\ mol \\ 2\ mol \end{bmatrix}$. Since the reaction scale does not consume any material from the economy scale, usptream cut-offs from economy scale (X_u^E) are 0. The sub-matrix A' representing this system is as follows,

$$A^r = V^{rT} - U^r = [1 \quad 2] - [0 \quad 0] = [1 \quad 2] \tag{A.2}$$

The corresponding representation of the reaction scale has been shown in figure A.2.

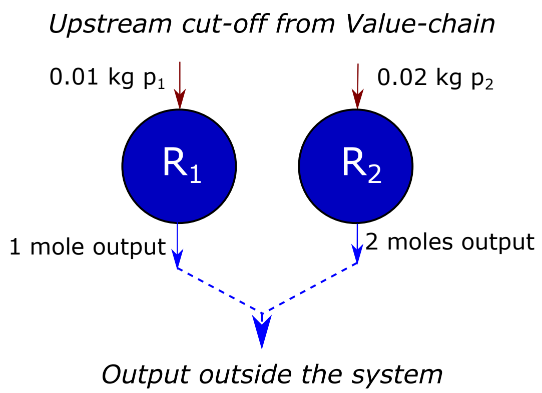

Figure A.2: Illustrative Example, Reaction scale inputs and outputs explained

A.2 Value Chain Scale

The make ($\underline{V}$) and use ($\underline{U}$) matrices of the value-chain are usually based on private or government databases such as Ecoinvent or NREL. These databases are developed by collecting data pertaining to various life-cycle activities such as electricity production, diesel production, incineration, etc. and publish regional or national averages of inputs and outputs to these processes. Often, data is published directly as the technology matrix $\underline{A}$. However, disaggregation equations in the P2P-RNFA framework require computations on the make and use matrices. In such cases, therefore, the technology matrix is decomposed into make and use matrices. This is done by considering only positive cells in the make matrix, and negative elements in the use matrix, thereby satisfying the relation $\underline{A} = \underline{V}^T - \underline{U}$. The make and use matrices for the illustrative example are as follows,

$$\text{Value-chain Scale} \quad \underline{V} = \begin{bmatrix} 35 & 0 \\ 0 & 50 \end{bmatrix} \quad \underline{U} = \begin{bmatrix} 15 & 7 \\ 5 & 10 \end{bmatrix} \quad \underline{B} = \begin{bmatrix} 4 & 20 \end{bmatrix} \tag{A.3}$$

Here, the first row corresponds to the flow of the product p_1, and second row corresponds to flow of p_2. The first column indicates the value-chain activity VC_1, whereas the second indicates VC_2. Make and use matrices (original or disaggregated) can be used to calculate the technology matrix $\underline{A}$ or $\underline{A}^*$ using the following relation: $\underline{A} = \underline{V}^T - \underline{U}$. This has been demonstrated for the illustrative example below,

$$\underline{A} = V^T - U = \begin{bmatrix} 35 & 0 \\ 0 & 50 \end{bmatrix} - \begin{bmatrix} 15 & 7 \\ 5 & 10 \end{bmatrix} = \begin{bmatrix} 20 & -7 \\ -5 & 40 \end{bmatrix} \tag{A.4}$$

Since the two reactions demand substances from the coarser value-chain scale, there exists an upstream cut-off, $X_u^V = \begin{bmatrix} 0.01\text{kg p}_1 & 0 \\ 0 & 0.02\text{kg p}_2 \end{bmatrix}$, as evident from figure A.3. Additionally, the value-chain demands inputs from the economy scale, i.e VC_1 requires 4\$ of commodities from E_2, and VC_2 demands 5\$ of commodities from E_2. Thus, the upstream cut-off corresponding to this is: $\underline{X}_u = \begin{bmatrix} \$4 & \$5 \\ 0 & 0 \end{bmatrix}$. Individually, each value-chain activity can be represented in the graph diagram using the make and use matrices as shown in figure A.3 (a), whereas the technology matrix and upstream cut-off flows can be used to describe the intra-scale flows as shown in figure A.3 (b). Notably, the downstream cut-offs from value-chain to economy scale are zero because there are no flows going back to the economy scale.

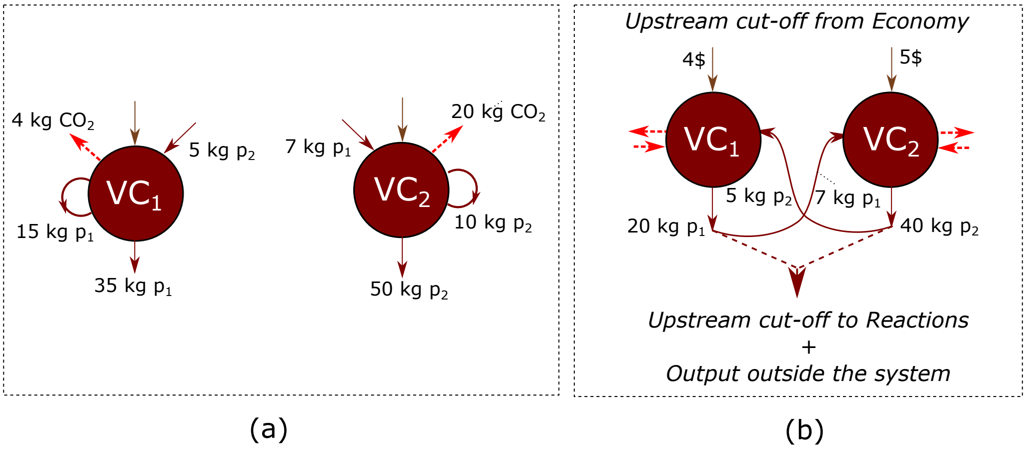

Figure A.3: Illustrative Example, Value-Chain scale inputs and outputs explained. (a) Individual value-chain activities modelled from make and use matrices (b) Value-chain scale network described using technology and cut-off matrices

A.3 Economy Scale

The economy scale make and use matrices of the Economic Input Output model are usually available from the government's trade and commerce websites. For example, the United States Bureau of Economic Analysis (US BEA) provides the economic flows between 385 industries within the economy, in the form of make and use matrices ($\overline{V}$ and $\overline{U}$). In the illustrative example, the economy scale make and use matrices are as follows,

$$\text{Economy Scale} \quad \overline{V} = \begin{bmatrix} \$500 & 0 \\ 0 & \$700 \end{bmatrix} \quad \overline{U} = \begin{bmatrix} \$150 & \$200 \\ \$300 & \$100 \end{bmatrix} \tag{A.5}$$

These numbers in $\overline{V}$ and $\overline{U}$ are depicted as flows in figure A.4 for both economic sectors E_1 and E_2. In the P2P-RNFA framework, make and use matrices from all the three scales are used to perform disaggregation. This yields corrected make and use matrices. The direct requirements matrix $\overline{A}$ and Leontief matrix, $I - \overline{A}$ of the economy scale are then computed from corrected make and use matrices using the following equation,

$$
\begin{aligned}
\overline{A} &= \overline{U}(\overline{V}^T)^{-1} = \begin{bmatrix} \$150 & \$200 \\ \$300 & \$100 \end{bmatrix} \left(\begin{bmatrix} \$500 & 0 \\ 0 & \$700 \end{bmatrix}^T \right)^{-1} = \begin{bmatrix} 0.300 & 0.286 \\ 0.600 & 0.143 \end{bmatrix} \\
I - \overline{A} &= \begin{bmatrix} 0.700 & -0.286 \\ -0.600 & 0.857 \end{bmatrix}
\end{aligned}
\tag{A.6}
$$

The direct requirements matrix can now be used to represent the economy scale flows. The environmentally-extended economic input-output model is used to quantify these flows as functions of industry throughputs (x) to meet the net outputs required from the economy scale. Balance of monetary flows is acheived using the Leontief equation $(I - \overline{A})\overline{x} = \overline{f}$ (final demand). Outputs from economy scale are either final demands outside the system of downstream cut-offs to the finer scales, i.e. value-chain and reaction scales. This has been depicted in figure A.4.

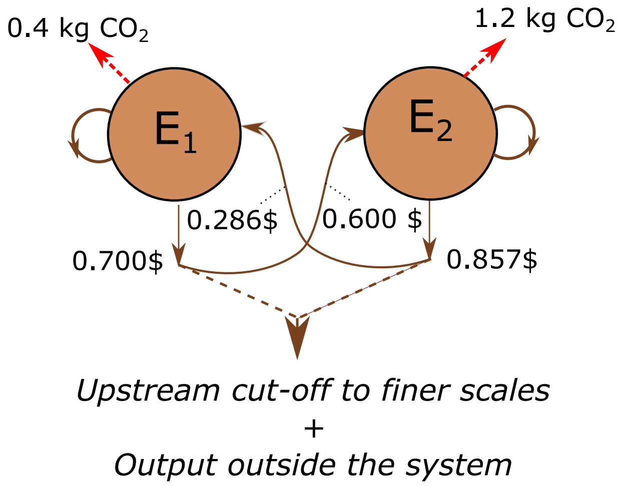

Figure A.4: Illustrative Example, Economy scale cash flows explained.

A.4 Integration of scales

In this tutorial, we omit the disaggregation aspect of the P2P-RNFA framework, and demonstrate how the matrices of individual scales and other parameteric matrices are used to construct a multi-scale matrix. Essentially, this involves substituting stoichiometric, technology and direct requirements matrices from previous sections on the diagonal elements, and cut-off matrices on the off-diagonal elements. The resulting multi-scale matrix is as follows,

$$
\begin{aligned}
\underline{\overline{X}} &= \begin{bmatrix} \overline{I} - \overline{A} & -\underline{X}_u & -X_u^E \\ -\underline{X}_d & \underline{A} & -X_u^V \\ -X_d^E & -X_d^V & A' \end{bmatrix} \\
] &= \begin{bmatrix} 0.700 & -0.286 & 0 & 0 & 0 & 0 \\ -0.600 & 0.857 & -4 & -5 & 0 & 0 \\ 0 & 0 & 20 & -7 & -0.01 & 0 \\ 0 & 0 & -5 & 40 & 0 & -0.02 \\ 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix}
\end{aligned}
\tag{A.7}
$$

If there exists disaggregation, the coarser scale matrices need to be corrected using equations 11 and 12 of the main paper. This requires permutation matrices, price vectors and process-product matrices. Consider the illustrative example in figure A.1 but with a disaggregation scheme as shown in figure A.5.

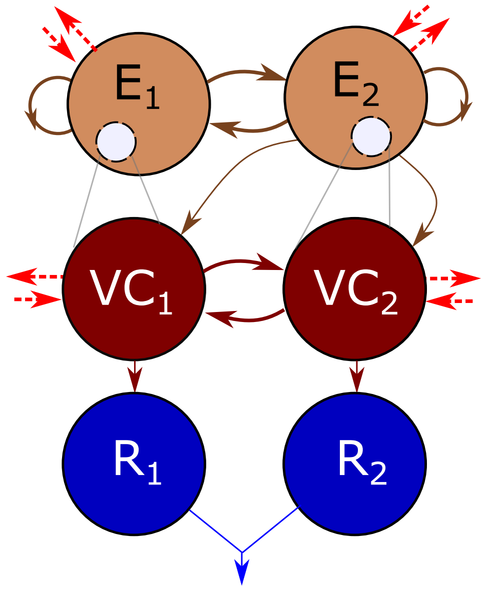

Figure A.5: Illustrative Example, Superstructure Network with disaggregation

In this illustration, VC_1 and its output product p_1 are disaggregated from economic sector E_1 due to overlap, i.e. product p_1 is also an output of E_1 and VC_1 is comprised in E_1. Similarly, VC_2 and its product p_2 are parts of economic sector E_2.

$$\text{Value-chain \& Economy} \quad \underline{P}_F = \begin{array}{c} \\ E_1 \\ E_2 \end{array}\begin{bmatrix} p_1 & p_2 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \underline{P}_P = \begin{array}{c} \\ VC_1 \\ VC_2 \end{array}\begin{bmatrix} E_1 & E_2 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{A.8}$$

The flow permutation matrix P_F contains cells assume value of 1 when an economic sector, indicated by the row, also produces a value-chain product indicated by the column. For the example in figure A.5, the economic sector E_1 also produces p_1 in addition to VC_1 whereas E_1 does not produce p_2, therefore matrix has value one for index E_1, p_1 whereas zero for E_1, p_2. The process permutation matrix P_P contains cells assume value of 1 when a value-chain process, indicated by the row, is part of the economic sector indicated by the column. For this illustration VC_1 is part of economic sector E_1 whereas VC_2 is not. Therefore the cell of matrix P_P referenced by VC_1, E_1 is one, whereas the one by VC_1, E_2 is zero. Since, the reaction scale is not to be disaggregated from the economy or value-chain scales in this example, permutation matrices for these pairings of scales are all zero, as shown below.

$$\begin{aligned} &\text{Reaction \& Economy} \quad \underline{P}_F^E = \begin{array}{c} \\ E_1 \\ E_2 \end{array}\begin{bmatrix} o/p \\ 0 \\ 0 \end{bmatrix} \quad \underline{P}_P^E = \begin{array}{c} \\ R_1 \\ R_2 \end{array}\begin{bmatrix} E_1 & E_2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \\ &\text{Reaction \& Value-Chain} \quad \underline{P}_F^V = \begin{array}{c} \\ VC_1 \\ VC_2 \end{array}\begin{bmatrix} o/p \\ 0 \\ 0 \end{bmatrix} \quad \underline{P}_P^V = \begin{array}{c} \\ R_1 \\ R_2 \end{array}\begin{bmatrix} VC_1 & VC_2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \end{aligned} \tag{A.9}$$

In addition to permutation matrices, disaggregation equations also require price vectors (p) which contain the price of value-chain products per kg. For this example, the price of both p_1 and p_2 is assumed to be 0.01\$/kg. Thus $p = [\begin{smallmatrix} p_1 & p_2 \\ 0.01\$ & 0.01\$ \end{smallmatrix}]$. The process-product matrix $\overline{P}$ is an identity matrix because product p_1 is part of value-chain process VC_1, whereas p_2 is part of VC_2. The process-product matrix for reaction scale is [1 1], since the output product is part of both reactions R_1 and R_2. These parameters can be used to perform disaggregation as shown in equations 11-12. It has been replicated here,

$$\begin{aligned}
\overline{V}^*(\{\underline{s}\}) &= \overline{V} - \hat{p}\left(\underline{P}_P\hat{\underline{s}}\right)^{\mathrm{T}} \underline{V}\left(\underline{P}_F\right)^{\mathrm{T}} - \hat{p}\left(P_P^E\hat{\underline{s}}\right)^{\mathrm{T}} V\left(P_F^E\right)^{\mathrm{T}} \\
\overline{U}^*(\{\underline{s}\}) &= \overline{U} - \left(\underline{P}_F\hat{p}\underline{U}\hat{\underline{s}}P_P + \underline{P}_F\overline{P}\hat{\underline{s}}\overline{P}^T\underline{p}\underline{X}_d + \underline{X}_u\hat{\underline{s}}P_P\right) \\
&\quad - \left(P_F^E\hat{p}U\hat{s^r}{P_P}^E + {P_F}^E P^r\hat{s^r}{P^r}^T\hat{p}X_d^E + X_u^E P_P^E\hat{s^r}\right)
\end{aligned} \tag{A.10}$$

The P2P-RNFA formulation in section 3.1.3 requires variable disaggregation, wherein the scaling ($\underline{s}$) and reaction extent vector (s^r) are variables and corrected make and use matrices are functions of these vectors. The multi-scale matrix elements are found as a function of these corrected matrices, as shown below.

$$\begin{aligned}
\overline{A}^*(\{\underline{s}, s^r\}) &= \overline{U}^*(\{\underline{s}, s^r\})[\overline{V}^{*T}(\{\underline{s}, s^r\})]^{-1} && \text{Direct requirements matrix} \\
\underline{A}^*(\{s^r\}) &= \underline{U}^*(\{s^r\}) - [\underline{V}^*(\{s^r\})]^T && \text{Technology Matrix} \\
A' &= V^T - U && \text{Stoichiometric Matrix}
\end{aligned} \tag{A.11}$$

These equations form the constraints of the P2P-RNFA formulation, with the scaling vectors and reaction extents being the decision variables. However, for the P2P-RNFA approximation algorithm, these corrected make and use matrices are found for each viable discreet pathway which satisfies all the other constraints. As a result, the corrected make and use matrices are parameteric. Equation A.11 involves simple matrix transformations and operations to find the multi-scale matrix. In the illustrative example, there are only two discreet pathways, and therefore it is easy to calculate the multi-scale matrix for the two pathways for a particular basis. Assuming 1000 moles of output from the system, the two multi-scale matrices corresponding to the two different pathways are as follows,

$$\begin{aligned}
&\text{Pathway 1:} \quad \underline{\overline{X}}_1 = \begin{bmatrix} \mathit{0.7005} & \mathit{-0.2857} & 0 & 0 & 0 & 0 \\ \mathit{-0.5960} & \mathit{0.8576} & -4 & -5 & 0 & 0 \\ 0 & 0 & 20 & -7 & -0.01 & 0 \\ 0 & 0 & -5 & 40 & 0 & -0.02 \\ 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix} \\
&] \\
&\text{Pathway 2:} \quad \underline{\overline{X}}_2 = \begin{bmatrix} \mathit{0.7000} & \mathit{-0.2858} & 0 & 0 & 0 & 0 \\ \mathit{-0.5992} & \mathit{0.8590} & -4 & -5 & 0 & 0 \\ 0 & 0 & 20 & -7 & -0.01 & 0 \\ 0 & 0 & -5 & 40 & 0 & -0.02 \\ 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix}
\end{aligned} \tag{A.12}$$

It can be noticed that due to variable disaggregation, the economy scale sub-matrix (in italics) are different for the two pathways, which are both different from the multi-scale matrix without disaggregation calculated in equation A.7. These matrices are identical to the ones used in equation 20 for the illustrative example. The difference between the two pathways becomes even more prominent when the basis increases resulting in larger overlap and bigger amounts of required disaggregation. These results are elaborated in the main paper.