II.11

a) The stoichiometric matrix S for this system will have 3 columns

b) S will have 5 rows

c)

$$S = \begin{bmatrix} -1 & 0 & 0 \\ -1 & 0 & -1 \\ 1 & -2 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 3 \end{bmatrix}$$

II.12

a) The reversible reaction v_4 was split into 2 irreversible reactions v_{4f} and v_{4r}. There are therefore a total of 6 compounds (ignoring A and AP) and 11 reactions, but the matrix below is 6×10 since the last reaction (v_7) only involves the compounds we are ignoring.

$$S = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

b) In the following equations, let $x_i := [x_i]$ for simplicity.

$$\begin{aligned} \frac{dx_1}{dt} &= b_1 - v_1 x_1 \\ \frac{dx_2}{dt} &= v_1 x_1 - v_2 x_2 - v_3 x_4 \\ \frac{dx_3}{dt} &= v_2 x_2 + v_{4r} x_4 - b_2 x_3 - v_{4f} x_3 \\ \frac{dx_4}{dt} &= v_3 x_2 + v_{4f} x_3 - v_{4r} x_4 - v_5 x_4 \\ \frac{dx_5}{dt} &= v_5 x_4 - v_6 x_5 \\ \frac{dx_6}{dt} &= v_6 x_5 - b_3 \end{aligned}$$

II.26

a)

- $$S = \begin{bmatrix} 1 & -1 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & -1 & 1 \end{bmatrix}$$

- $$null(S) = \begin{bmatrix} 0.5682 & -0.5682 & -0.1023 & 0.1023 \\ 0.1955 & -0.1955 & -0.5432 & 0.5432 \\ 0.6864 & 0.3136 & 0.2205 & -0.2205 \\ 0.3136 & 0.6864 & -0.2205 & 0.2205 \\ 0.1864 & -0.1864 & 0.7205 & 0.2795 \\ -0.1864 & 0.1864 & 0.2795 & 0.7205 \end{bmatrix}$$

- $$patmat(S) = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}$$

b)
- $$S = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 1 \end{bmatrix}$$
- $$null(S) = \begin{bmatrix} 0.7370 & -0.2024 & 0.2024 \\ 0.2132 & -0.5383 & 0.5383 \\ 0.5237 & 0.3359 & -0.3359 \\ 0.2619 & 0.6680 & 0.3320 \\ -0.2619 & 0.3320 & 0.6680 \end{bmatrix}$$
- $$patmat(S) = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

c)
- $$S = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$
- $$null(S) = \begin{bmatrix} -0.0979 & 0.4174 & -0.4174 & 0.1164 & -0.1164 & 0.1721 & -0.1721 \\ 0.1638 & 0.2968 & -0.2968 & 0.2742 & -0.2742 & -0.2133 & 0.2133 \\ 0.1046 & 0.2603 & -0.2603 & -0.4798 & 0.4798 & 0.0459 & -0.0459 \\ 0.3663 & 0.1397 & -0.1397 & -0.3220 & 0.3220 & -0.3395 & 0.3395 \\ 0.4741 & 0.0120 & -0.0120 & -0.0156 & 0.0156 & 0.4391 & -0.4391 \\ 0.7357 & -0.1086 & 0.1086 & 0.1422 & -0.1422 & 0.0537 & -0.0537 \\ -0.0489 & 0.7087 & 0.2913 & 0.0582 & -0.0582 & 0.0861 & -0.0861 \\ 0.0489 & 0.2913 & 0.7087 & -0.0582 & 0.0582 & -0.0861 & 0.0861 \\ 0.0819 & 0.1484 & -0.1484 & 0.6371 & 0.3629 & -0.1066 & 0.1066 \\ -0.0819 & -0.1484 & 0.1484 & 0.3629 & 0.6371 & 0.1066 & -0.1066 \\ -0.1308 & 0.0603 & -0.0603 & -0.0789 & 0.0789 & 0.6927 & 0.3073 \\ 0.1308 & -0.0603 & 0.0603 & 0.0789 & -0.0789 & 0.3073 & 0.6927 \end{bmatrix}$$
- $$patmat(S) = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}$$

d) .

II.27

a) The following network has 3 extreme pathways.

$$S = \begin{bmatrix} 1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & -1 \end{bmatrix}$$

b) The following network has 9 extreme pathways.

$$S = \begin{bmatrix} 1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & -1 \end{bmatrix}$$

c) For $n = 3$ there are 27 extreme pathways. In general, the number of extreme pathways in a network based on this model is 3^n. In general, you expect the number of extreme pathways to grow more subtly as the number of reactions increases.