PS3

a)

Metabolites:

1	ATP	10	citrulline
2	AMP	11	argininosuccinate
3	Diphosphate	12	arginine
4	phosphate	13	ornithine
5	H_2O	14	NADPH
6	Carbamoyl Phosphate	15	H^+
7	Aspartate	16	O_2
8	Fumarate	17	NO
9	urea	18	$NADP^+$

Fluxes:

v1: $ATP + Citru + Aspar \rightarrow AMP + diphos + succi$

v2: $succi \rightarrow fumar + argin$

v3: $argin + H_2O \rightarrow ornith + urea$

v4: $carbamoyl + ornith \rightarrow phosph + citru$

v51: $argin + 1.5NADPH + 1.5\,H^+ + 2O2 \rightarrow citru + NO + 1.5NADP + 2H_2O$

v52: $citru + NO + 1.5NADP + 2H_2O \rightarrow argin + 1.5NADPH + 1.5\,H^+ + 2O2$

b1: $source \rightarrow carbamoyl$

b2: $source \rightarrow aspar$

b3: $fumar \rightarrow sink$

b4: $urea \rightarrow sink$

b5: $source \rightarrow ATP$

b6: $source \rightarrow water$

b7: $diphos \rightarrow sink$

b8: $phos \rightarrow sink$

b9: $AMP \rightarrow sink$

b10: $source \rightarrow NADPH$

b11: $source \rightarrow H^+$

b12: $source \rightarrow O_2$

b13: $NO \rightarrow sink$

b14: $source \rightarrow NADP^+$

Stoichiometric matrix: Rows are metabolites and columns are fluxes.

s =

-1.0000	0	0	0	0	0	0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0	0
1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	-1.0000	0	0	0	0	0	0
1.0000	0	0	0	0	0	0	0	0	0	0	0	-1.0000	0	0	0	0	0	0	0	0
0	0	0	1.0000	0	0	0	0	0	0	0	0	0	-1.0000	0	0	0	0	0	0	0
0	0	-1.0000	0	2.0000	-2.0000	0	0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0
0	0	0	-1.0000	0	0	1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.0000	0	0	0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1.0000	0	0	0	0	0	0	-1.0000	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1.0000	0	0	0	0	0	0	-1.0000	0	0	0	0	0	0	0	0	0	0	0
-1.0000	0	0	1.0000	1.0000	-1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1.0000	-1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1.0000	-1.0000	0	-1.0000	1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1.0000	-1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	-1.5000	1.5000	0	0	0	0	0	0	0	0	0	1.0000	0	0	0	0	0
0	0	0	0	-1.5000	1.5000	0	0	0	0	0	0	0	0	0	0	1.0000	0	0	0	0
0	0	0	0	-2.0000	2.0000	0	0	0	0	0	0	0	0	0	0	0	1.0000	0	0	0
0	0	0	0	1.0000	-1.0000	0	0	0	0	0	0	0	0	0	0	0	0	-1.0000	0	0
0	0	0	0	1.5000	-1.5000	0	0	0	0	0	0	0	0	0	0	0	0	0	-1.0000	0

b)

Atom matrix: The rows are C, H, N, O, P respectively, and the columns are

10	10	0	0	0	1	4	4	1	6	10	6	5	21	0	0	0	21
16	14	4	3	2	4	7	4	4	13	18	14	12	30	1	0	0	29
5	5	0	0	0	1	1	0	2	3	4	4	2	7	0	0	1	7
13	7	7	4	1	5	4	4	1	3	6	2	2	17	0	2	1	17
3	1	2	1	0	1	0	0	0	0	0	0	0	3	0	0	0	3

metabolites 1~18.

A*S=E

E =

0	0	0	0	0	0	1	4	−4	−1	10	0	0	0	−10	21	0	0	0	−21
0	0	0	0	0	0	4	7	−4	−4	16	2	−4	−3	−14	30	1	0	0	−29
0	0	0	0	0	0	1	1	0	−2	5	0	0	0	−5	7	0	0	−1	−7
0	0	0	0	0	0	5	4	−4	−1	13	1	−7	−4	−7	17	0	2	−1	−17
0	0	0	0	0	0	1	0	0	0	3	0	−2	−1	−1	3	0	0	0	−3

From Matlab, we can get E which is shown below.

From E, we can see that there are zeroes on the first 6 columns(for v1~v52).

Therefore, it's elementally balanced for the fluxes.

c)

The goal is to calculate the maximum rate of urea production. To do so, we need to calculate the upper bounds of each flux.

Using the formula from lecture note:

$0 \leq v \leq Vmax * theta * \left(\frac{a}{a+Km}\right)$, where Vmax=k_cat*E

and the bound from the problem set:

$0 \leq bj \leq \frac{10mmol}{gDW-hr}$

After calculating these bound values, we further use Flux.jl that solves the FBA problem to get the returned flux vector and also maximum urea flux which is 657.56 miumol/gDW-hr.