

Flux Balance Analysis (FBA)

Parker Poole, Environmental Engineering

Dr. Arul Varman

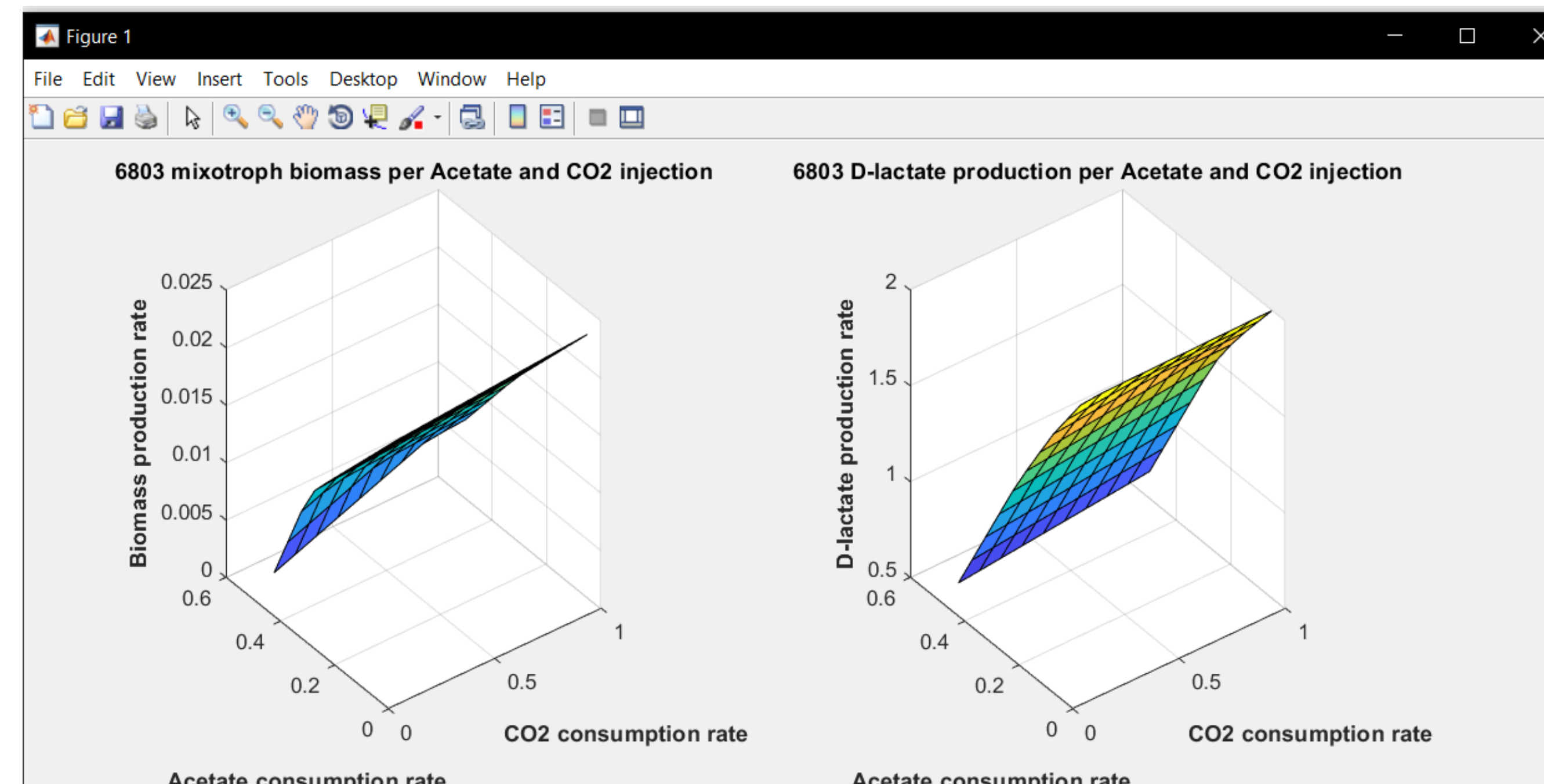
SEMTE

Flux Balance Analysis of *Synechocystis* sp. PCC 6803 for D-lactate production under mixotrophic conditions

Findings and progress thus far

```

Editor - C:\Users\pmanp\Documents\parkertry15.m
parkertry15.m  nimatry2.m  +
16 - for i = -.1:-.1:-1
17 -     x=x+1;
18 -     y = 0;
19 -     for j = -.05:-.05:-.5
20 -         y=y+1;
21 -         %model = changeRxnBounds(model, {'CO2tex'}, i, 'b');
22 -         %model = changeRxnBounds(model, {'ACTex'}, j, 'b');
23 -         model = changeRxnBounds(model, {'EX_o2_e'}, -1000, 'l');
24 -         model = changeRxnBounds(model, {'EX_co2_e'}, i, 'b');
25 -         model = changeRxnBounds(model, {'EX_ac_e'}, j, 'b');
26 -
27 -     model = changeObjective(model, {'BIOMASS_Ec_SynAuto'});
28 -     FBAsolution1 = optimizeCbModel(model, 'max');
29 -     %FBAsolution1 = relaxFBA(model, relaxOption);
30 -     FBAsolution1.f; % value of objective function (model.c'*F
31 -     FBAsolution1.v; % optimal solution vector
32 -     fluxData = FBAsolution1.v;
    
```



Command Window

CITt_kt	-0.525
Htex	-3.05
EX_mal__L_e	0.9875
HEX1	0.85
H2Otp	0.5125
CY01b2pp_syn	1.55
ATPS4rpp_1	0.7902
NDH1_4pp	1
NDH1_2p	0.55
PFK_3	0.6875
CBFCpp	1.55

fx >>

Obstacles

-Learning FBA programming

-Conceptual understanding of metabolic pathways

Biomass and lactate production per CO₂ and acetate injection (in progress)

Fluxes of certain reactions computed (mmol * gDW⁻¹ * hr⁻¹)

Spreadsheet of metabolic reactions used in code

rxn	rxn name	met
'ATPM'	'ATP maintenance requirement'	'23dhmb_c'
'CRBNTD'	'H2CO3 dissociation'	'23dhmp_c'
'NH3c'	'Ammonium proton dissociation'	'23dmpoh_c'
'MGDGE160'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C16 0)'	'lipidX_c'
'MGDGE161'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C16 1)'	'25aics_c'
'MGDGE180'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 0)'	'orn_c'
'MGDGE181'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 1)'	'25dhpp_c'
'MGDGE181_9'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 1)'	'26dap_LL_c'
'MGDGE182_9_12'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 2)'	'26dap_M_c'
'MGDGE183_6_9_12'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 3)'	'2a3o4pob_c'
'MGDGE183_9_12_15'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 3)'	'2ahbut_c'
'MGDGE184_6_9_12_15'	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 4)'	'2ahhmd_c'
'HSERTA'	'Homoserine O trans acetylase'	'2ahhmp_c'
'DDPA'	'3-deoxy-D-arabino-heptulosonate 7-phosphate synthetase'	'glcglyc_p_c'
'AHSERL2'	'O acetylhomoserine thiol lyase'	'glcglyc_c'
'DHQS'	'3-dehydroquinate synthase'	'glcglyc_p'
'DHQTI'	'3-dehydroquinate dehydratase, irreversible'	'glcglyc_e'

optimal	current	rxn name
-0.5	-0.5	'ATP maintenance requirement'
0	0	'H2CO3 dissociation'
0	0	'Ammonium proton dissociation'
3.53E-06	3.53E-06	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C16 0)'
-3.08E-05	-3.08E-05	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C16 1)'
0.000866	0.000866	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 0)'
0	0	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 1)'
6.51E-05	6.51E-05	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 1)'
0.00284	0.00284	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 2)'
0	0	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 3)'
0.00269	0.00269	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 3)'
0.00015	0.00015	'1,2-diacylglycerol 3-beta-D-glucose epimerase(n-C18 4)'
0.00269	0.00269	'Homoserine O trans acetylase'
0.00015	0.00015	'3-deoxy-D-arabino-heptulosonate 7-phosphate synthetase'
0	0	'O acetylhomoserine thiol lyase'
0.008524	0.008524	'3-dehydroquinate synthase'
0.002	0.002	'3-dehydroquinate dehydratase, irreversible'
0.00015	0.00015	'Adenosylmethionine decarboxylase'

Comparing optimal fluxes with calculated results

Acknowledgements

-Nima Hajinajaf, who mentored me on FBA