Outline for ARPA-E Update

* We have added more information to our model and reformatted it. The addition of ChEBI identifiers, plus the standardization of IDs in place of names for compounds, allows us to integrate more easily with other tools, such as the DOE Kbase, and also makes it easier for future updates.
* We fixed some GPR-relationship issues that were causing problems and comparing with the Whitman lab paper from 2013, we’re getting about 65% accuracy and an MCC of ~0.32, which aren’t ridiculously terrible considering we can’t account for polar effects and the gene function paper was a proxy, not a straight-on knockout experiment.
* We did an analysis of subsystems that are gapfilled and have a figure showing what these reactions are. We see meaningful trends here, particularly that a lot of these are hypothetical pathways from literature, covering about 46% of these 85 reactions. This means that of our ~700 reactions, about 7% of them are truly gapfilled. Half of the truly gapfilled ones are vitamin/cofactor syntheses or lack any subsystem.
* We’ve written our model up into a manuscript that we’re currently editing for submission. The manuscript highlights our model’s high gene homology, good degree of predictability for knockouts, addition of thermodynamics, and large amount of biochemical information from literature.
* We’ve done a sensitivity analysis on equilibrium quotient versus free energy prediction and found that, for the proposed stoichiometric solution to reversing methanogenesis, we’d need a value smaller than 10^-142 in order to drive the overall reaction in reverse. This further points to the idea that we’ll need to do more than close the stoichiometric loop.
* Our strain designs are a work in progress, we’ve run into some problems with the solver that are requiring some troubleshooting. This will be completed in the next couple weeks and we’re going to iteratively run through our solving process.
* We received our equipment and are working to confirm final numbers for dry cell weight v. optical density and ATP maintenance coefficients.
* By the end of the year, we will have some more strain designs, a submitted manuscript for the model, and confirmed quantitative measures for maintenance and growth yields.