MATLAB, Simulink, and Cantera for Aerospace Thermodynamic System Modeling

Joshua E. Freeh, Ananda Himansu, Christopher J. Steffen, Jr.,
Robert T. Tornabene, and Xiao-yen J. Wang
NASA Glenn Research Center
Cleveland, OH

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MATLAB, Simulink, and Cantera

MATLAB

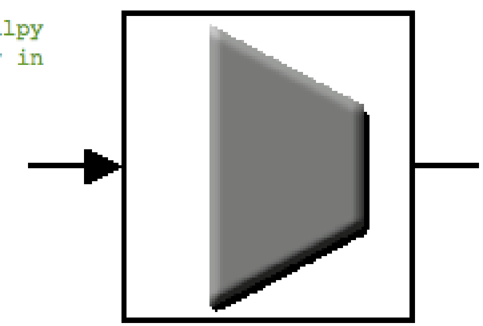
File Edit Text Go Cell Tools Debug

```
function u_out = compressor(u_in)
global nsp data

T_in = u_in(1);
P_in = u_in(2);
W_in = u_in(3);
X_in = u_in(4:nsp+3);

```

Cantera

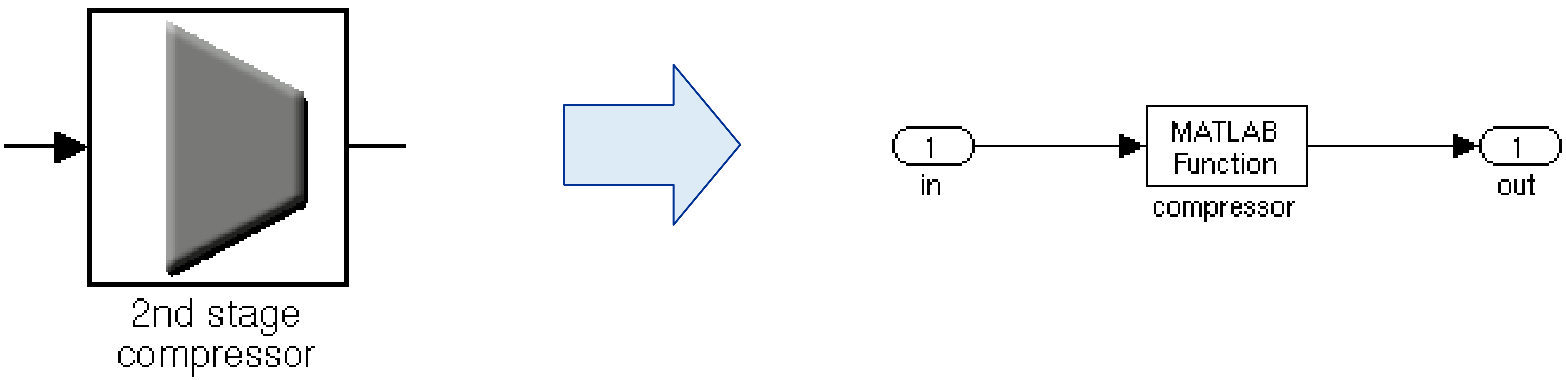
```
set(data.compressor.in.gas,'T',T_in,'P',P_in,'X',X_in);
data.compressor.in.W = W_in;

set(data.compressor.out.gas,'T',T_in,'P',P_in,'X',X_in);
data.compressor.out.W = data.compressor.in.W;

Pt_out = data.compressor.PR * pressure(data.compressor.i
 
Ht_in = enthalpy_mass(data.compressor.in.gas); %enthalpy
S_in = entropy_mass(data.compressor.in.gas); %entropy in
```

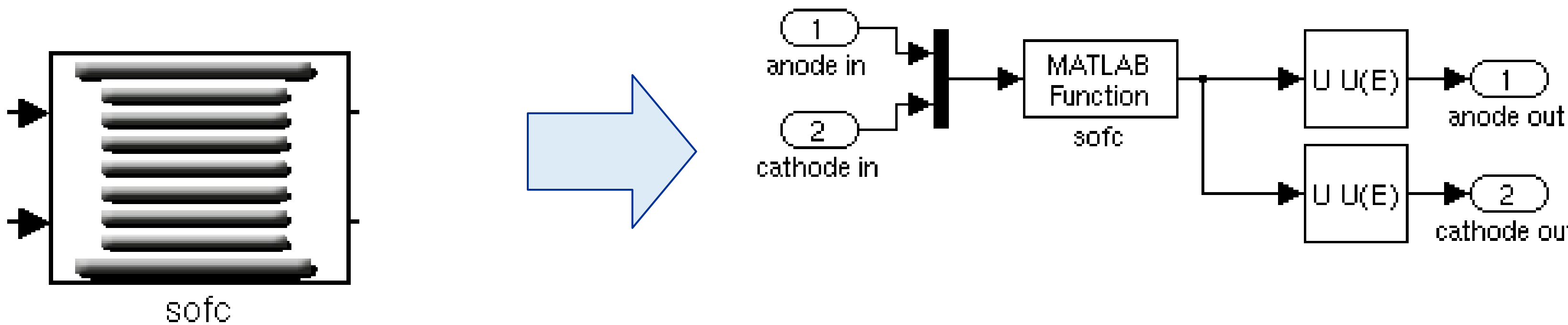
Simulink



2nd stage compressor

Simulink


2nd stage
compressor
1
in
MATLAB
Function
compressor
1
out


sofc
1
anode in
2
cathode in
MATLAB
Function
sofc
U U(E)
U U(E)
1
anode out
2
cathode out

…and MATLAB again

- `fmincon, fminbnd, fsolve`
  - Overall optimizers and nonlinear equation solvers
  - Minimize system mass or ensure conservation equations
- `gatool, patternsearch`
  - Non-gradient optimizers, though not necessary for current UAV model

Also…

- structures
  - Minimize variable handling and clarifies code
  - for example, `compressor.in.W` (or `.gas`, `.PR`, `.pwr`)

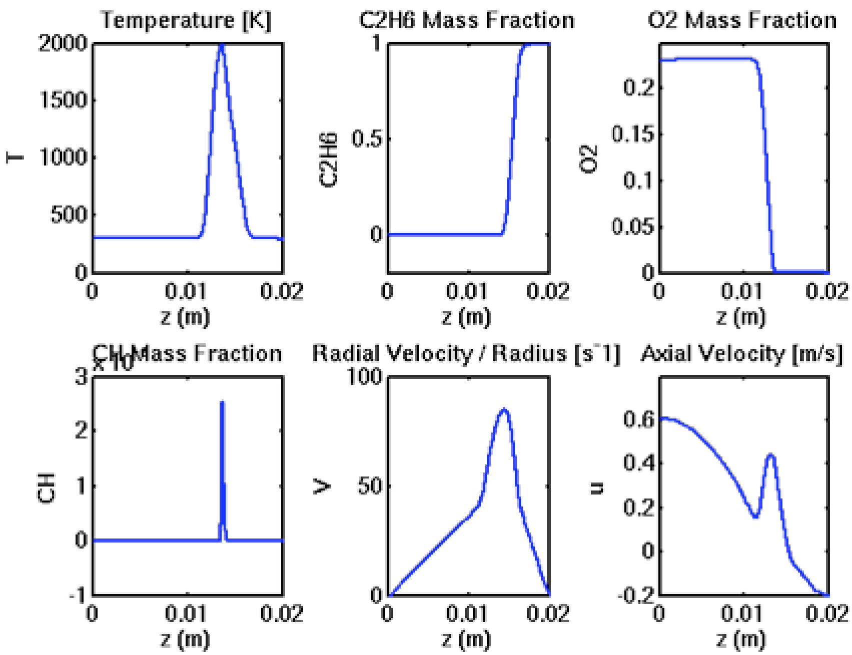
Cantera
(www.cantera.org)

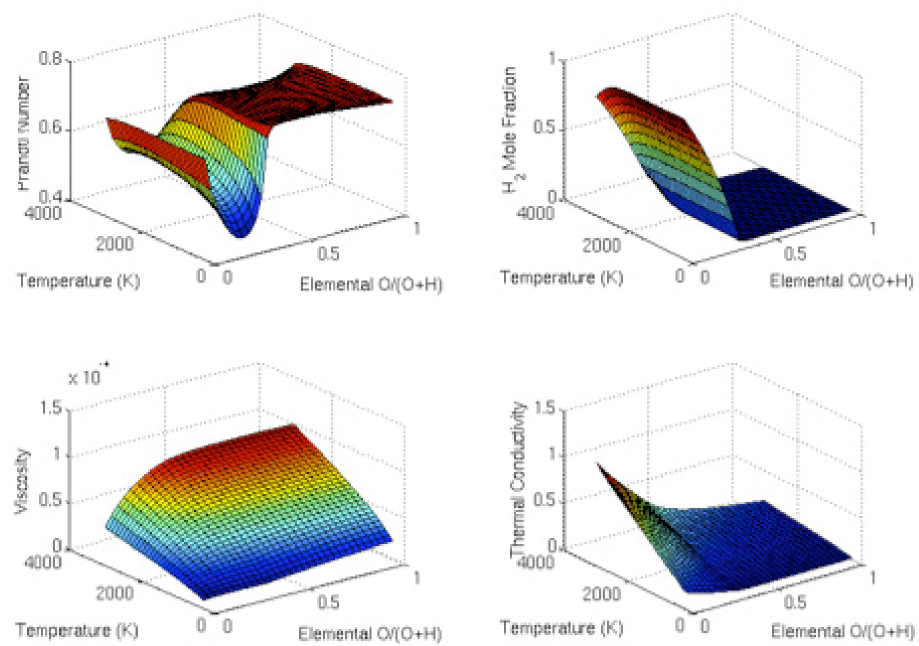
- Developed by David G. Goodwin, Professor of Mechanical Engineering and Applied Physics at California Institute of Technology

- Open source chemical reaction code
  - Written in C++
    - Compatible with MATLAB, Python, Fortran

- Capabilities
  - Thermodynamic and transport properties
  - Chemical equilibrium
  - Chemical kinetics
  - Electrochemistry
  - Pure substance equations of state
  - Others…

Cantera


Temperature [K]
T
z (m)
C2H6 Mass Fraction
C2H6
z (m)
O2 Mass Fraction
O2
z (m)
CH Mass Fraction
CH
z (m)
Radial Velocity / Radius [s^-1]
V
z (m)
Axial Velocity [m/s]
u
z (m)


Prandtl Number
Temperature (K)
Elemental O/(O+H)
H2 Mole Fraction
Temperature (K)
Elemental O/(O+H)
Viscosity
Temperature (K)
Elemental O/(O+H)
Thermal Conductivity
Temperature (K)
Elemental O/(O+H)

Cantera

MATLAB

```
gas = GRI30;
set(gas,'T',300.0,'P',OneAtm,'X','CH4:1,O2:2,N2:7.52');
equilibrate(gas,'HP');
disp(gas)
```

Python

```
from Cantera import *
gas = GRI30()
gas.set(T = 300.0, P = OneAtm, X = 'CH4:1,O2:2,N2:7.52')
gas.equilibrate('HP')
print gas
```

C++

```
#include "Cantera.h"
#include "GRI30.h"
#include "equilibrium.h"

main() {
    GRI30 gas;
    gas.setState_TPX(300.0, OneAtm, "CH4:1,O2:2,N2:7.52");
    equilibrate(gas, "HP");
    cout << gas;
}
```

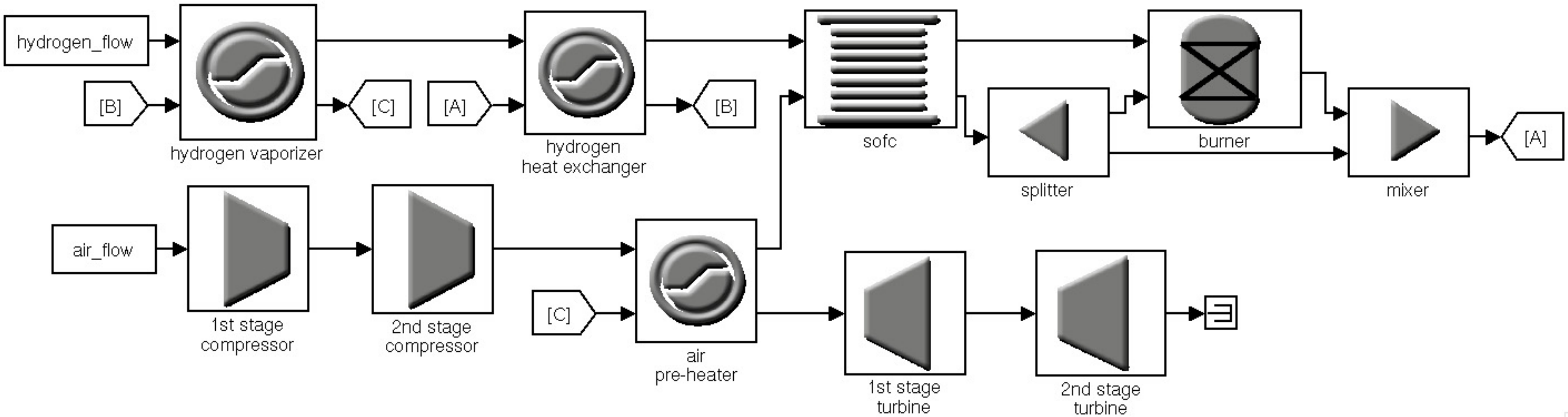
Objective

- Design a representative hybrid solid oxide fuel cell power system for high-altitude, long-endurance flight

- Understand the effect of major variables on the system
  - system level variables: altitude, power level, duration
  - component level variables: efficiencies, fuel cell resistivity

- Optimize system design
  - Current figure of merit: minimize mass

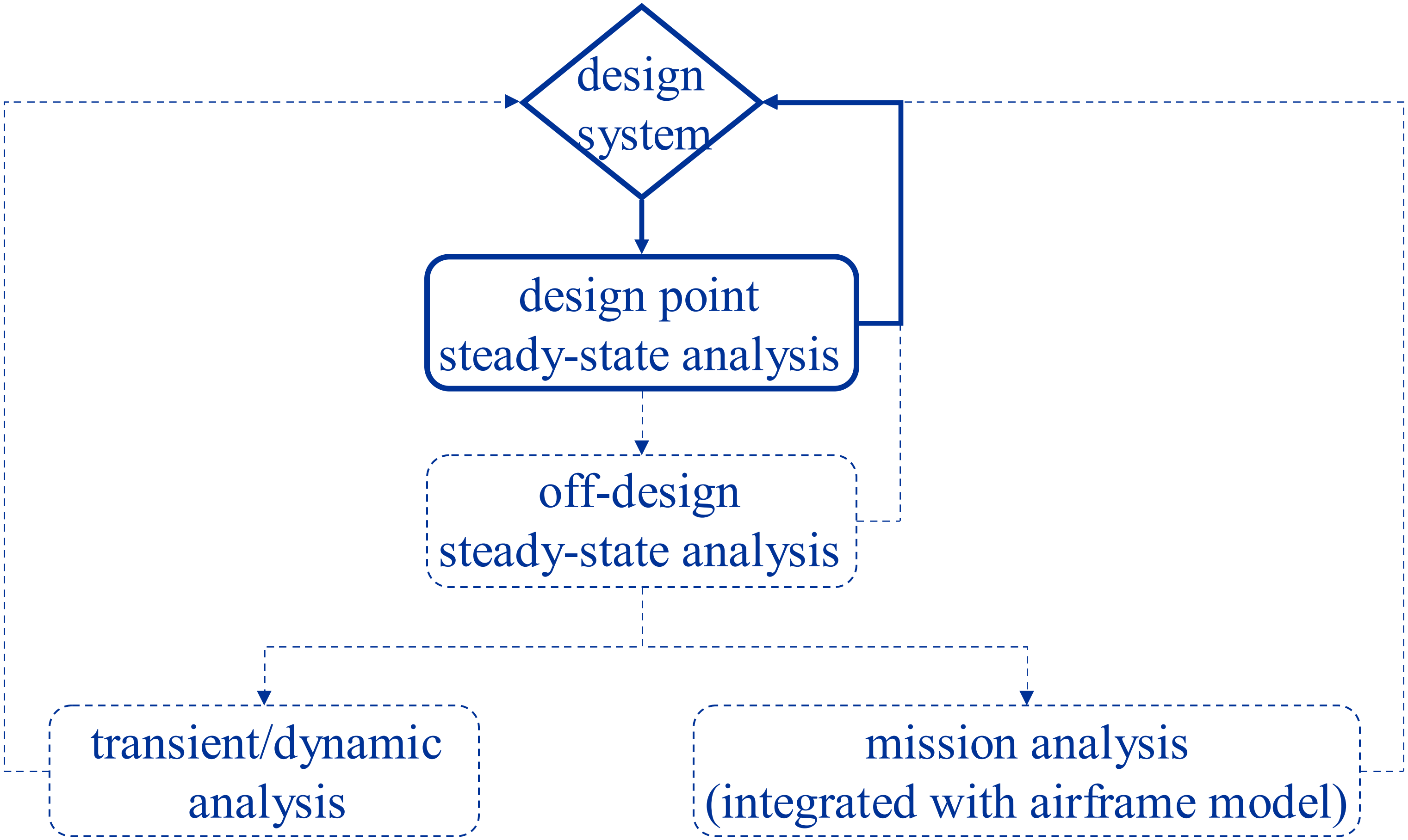
UAV power system



UAV power system specifications

- Baseline system
  - 21 km altitude (68,897 ft)
  - 50 kW net electrical power
  - η_{ad} = 0.8 for compressor stage, 0.85 for turbine stage
  - 2 stage radial turbomachinery designs
  - Planar solid-oxide fuel cell
    - 700°C inlet temperature, 1 atm inlet pressure
    - 100°C temperature increase across stack (air-cooled)
    - Maximum of 25 cells per stack, 25 cm^2 single cell active area
- Variations:
  - Altitude: 16 km
  - Power: 20 kW
  - Sensitivities on compressor and turbine η_{ad}, fuel cell ASR and stack design

Assumptions and Limitations



Past studies

Previous work (most undocumented)

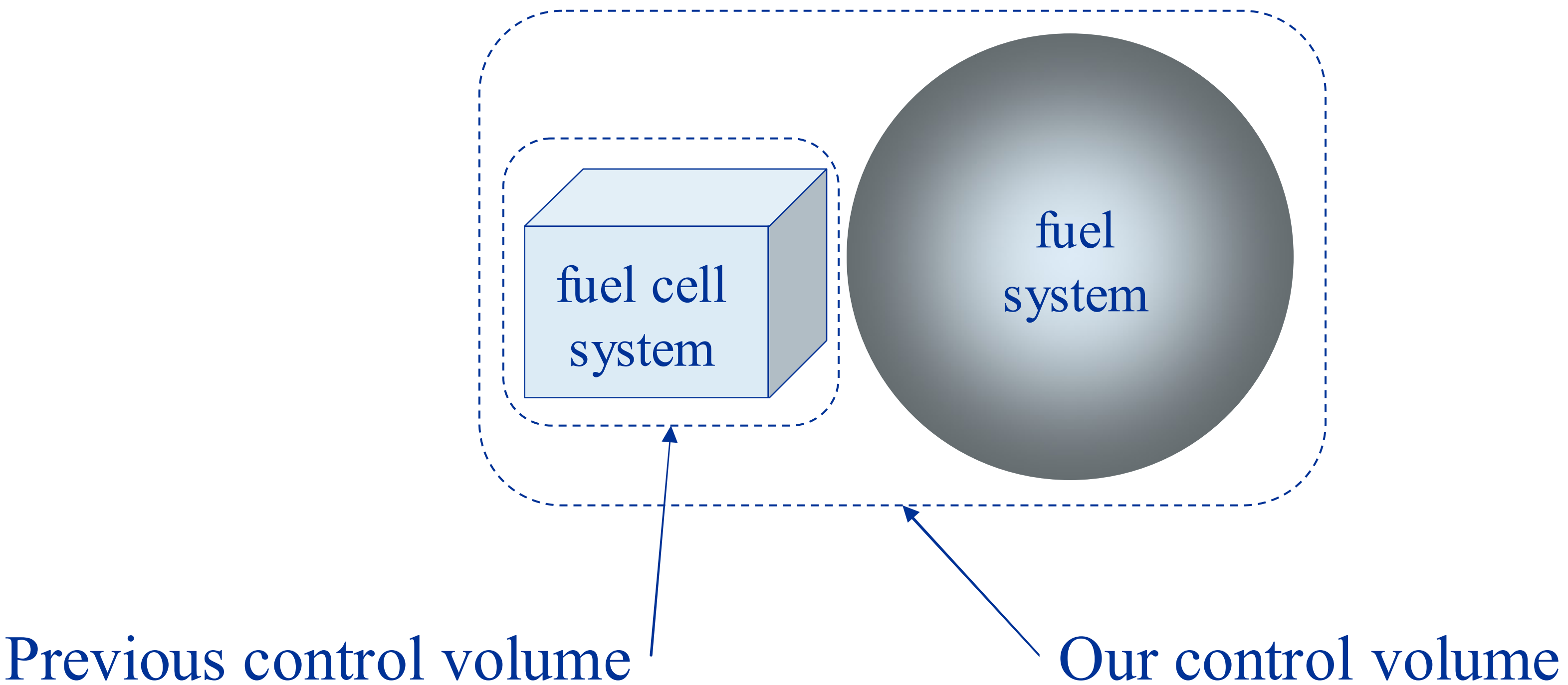
Minimize

fuel cell system mass

Our work

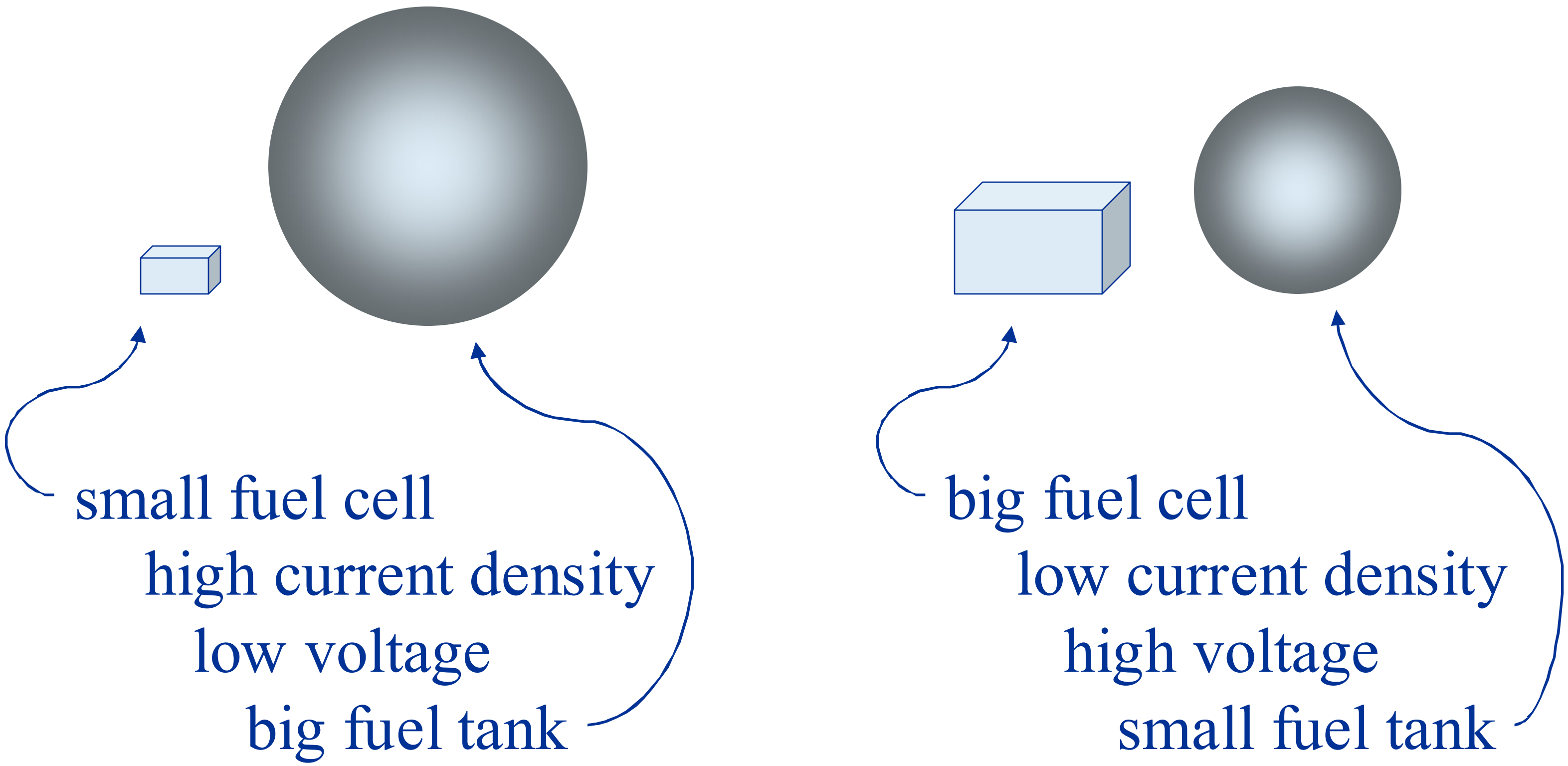
Minimize

(fuel cell system + fuel system) mass



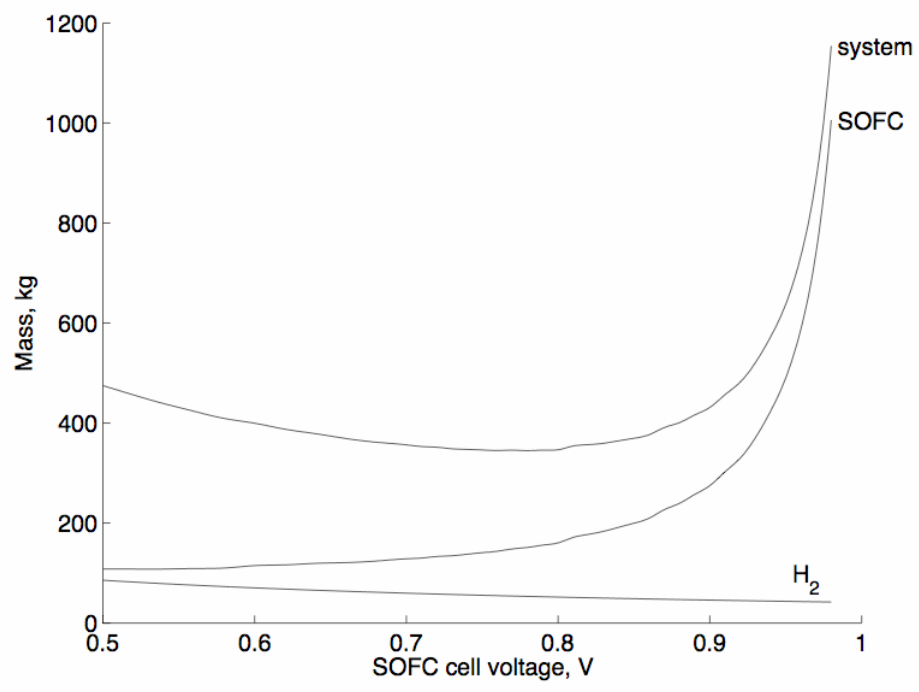
Qualitative (pre)analysis

for constant fuel cell power,

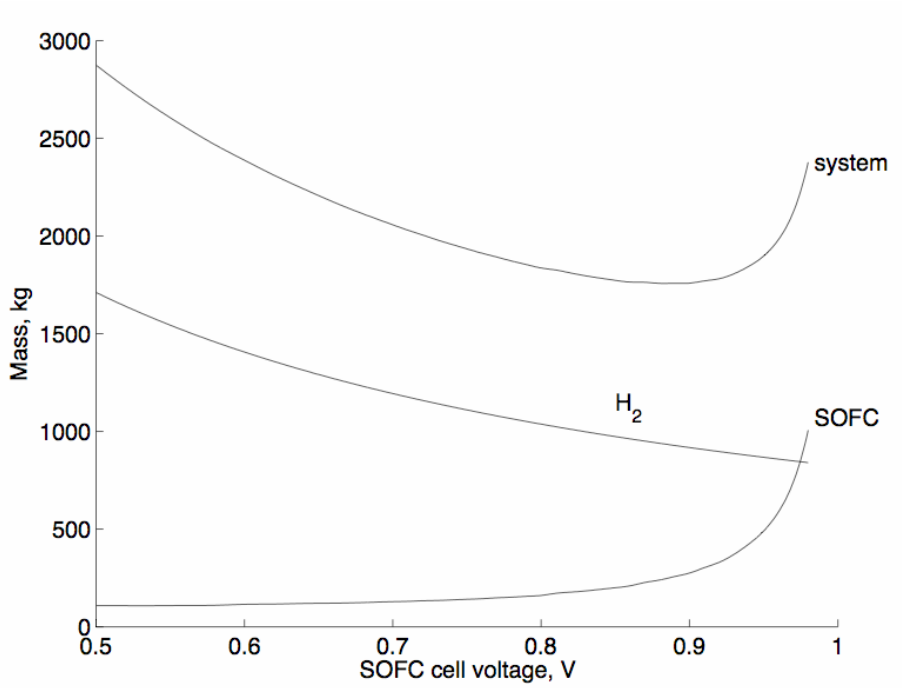


∴ there is a optimum system that minimizes mass/volume

Effect of mission duration



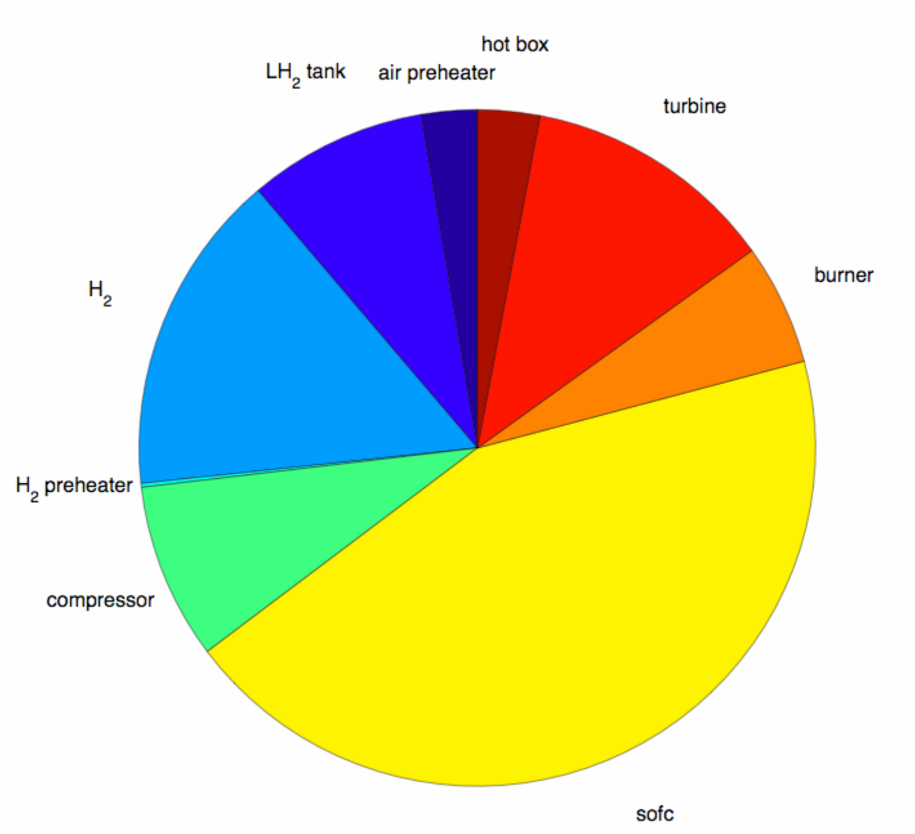
1 day mission



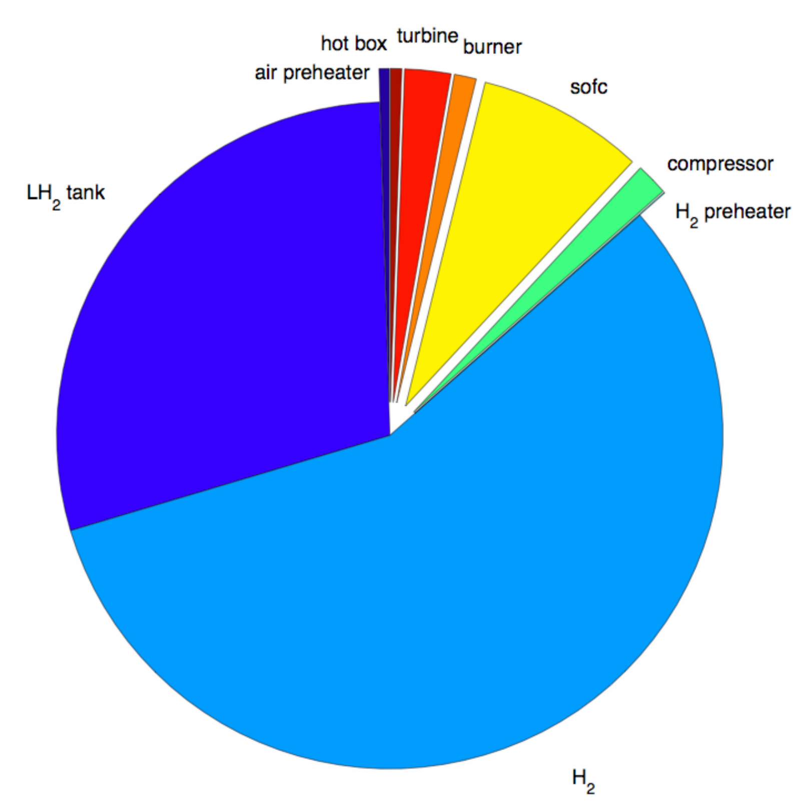
20 day mission

Another view of mission duration

(using optimum solutions from previous plots)

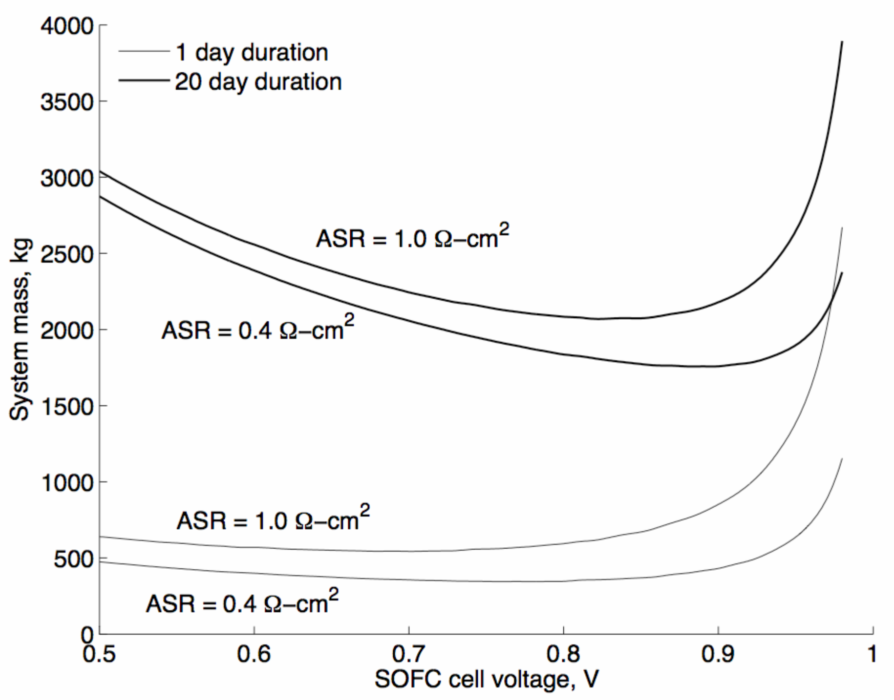


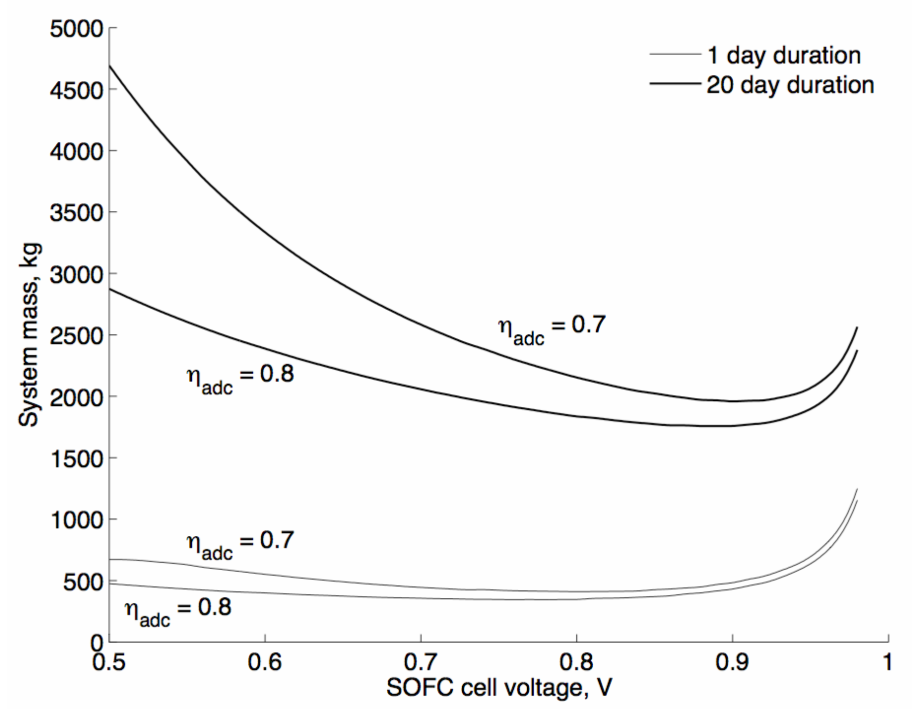
1 day mission



20 day mission

Sensitivity studies





Conclusions

- Combination of MATLAB, Simulink, and Cantera
  - Flexible and customizable interface
    - Currently using similar approach for lunar oxygen production system analysis
  - Scalable analysis capability
    - Cantera offers much more than currently being used here
    - MATLAB/Simulink as well
      - other toolboxes
        - » Statistics, SimPowerSystems
      - Also full capability of Simulink
        - » Dynamic and transient modeling

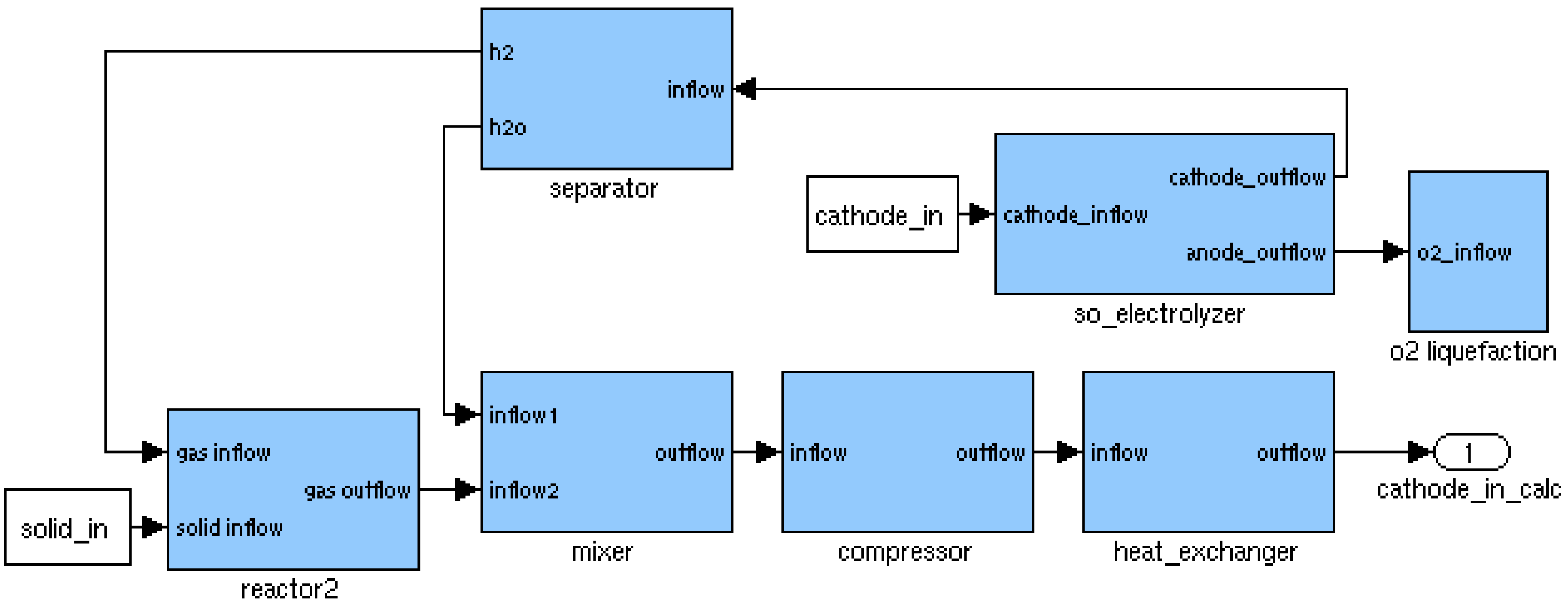
- UAV fuel cell system is possible when analyzed at the correct system level
  - especially for this application (high altitude, long endurance)

More information on this work

- Results will be presented in more detail on June 19
  - ASME Fuel Cell Science, Engineering, and Technology Conference in Irvine, CA
    - Paper # FUELCELL2006-97095

- Also available as a NASA Technical Memorandum
  - NASA TM-2006-214328
  - (will be online soon at http://ntrs.nasa.gov)

Lunar O_2 production model



Recommendations

- There is a better way to integrate these codes *(though we haven't found it yet)*
- Simulink can only pass numerical signals
  - Structures (with different data types) would help
  - Cantera objects (pointers?) would be even better
- More focus on Simulink as a steady-state tool
  - e.g. more flexibility and power with algebraic loop solver
    - Currently using MATLAB's `fsolve` to balance system .mdl
- Most of the current analysis time is interacting between three codes
  - Simulink-native (S-functions?) Cantera would help
  - Better S-function documentation or examples would help move this along

Thanks!

Contact information

Josh Freeh

NASA Glenn Research Center

(216) 433-5014

joshua.e.freeh@nasa.gov

Recommendations

- Cantera/mex interface does not always build correctly
  - May be a Cantera issue
  - and/or mex issue
  - and/or Macintosh issue (different versions of gcc, Tiger, etc.)

- Macintosh version can be much better

  (although some of these issues go beyond the scope of The MathWorks)
  - Can be much more than just a Unix/X11 port
  - Native Aqua, Quartz and other Mac-specific features
  - Use of AltiVec capabilities
  - Better Excel interface
  - Automatic local parallelization (for multi-processor machines)
  - XGrid