Current Density in the Mark IV with Cadmium Pool

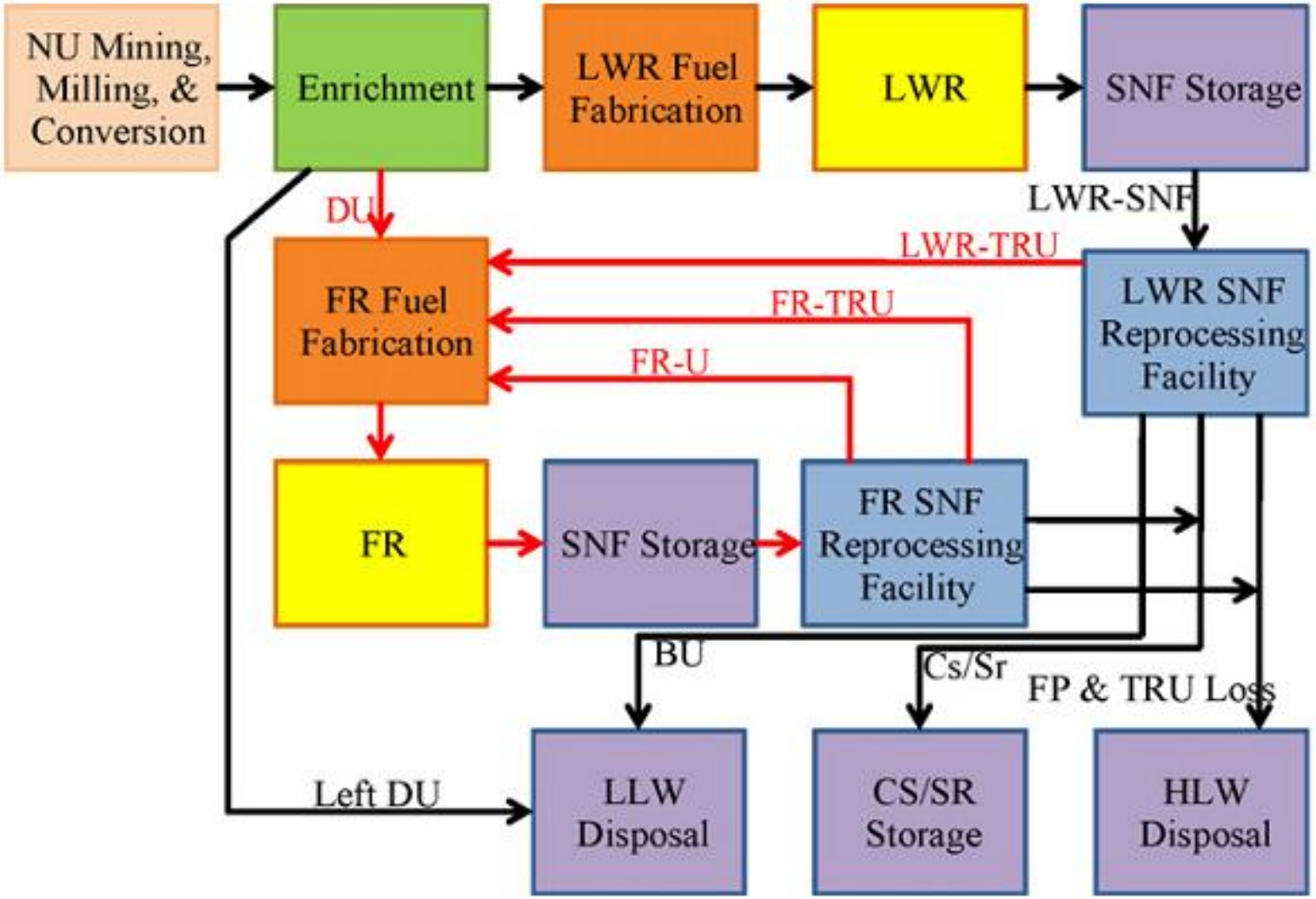
Jun Li, David McNelis

Aug 26-29, 2012

IPRC 2012

UNC
INSTITUTE FOR
THE ENVIRONMENT

Advanced Fuel Cycle

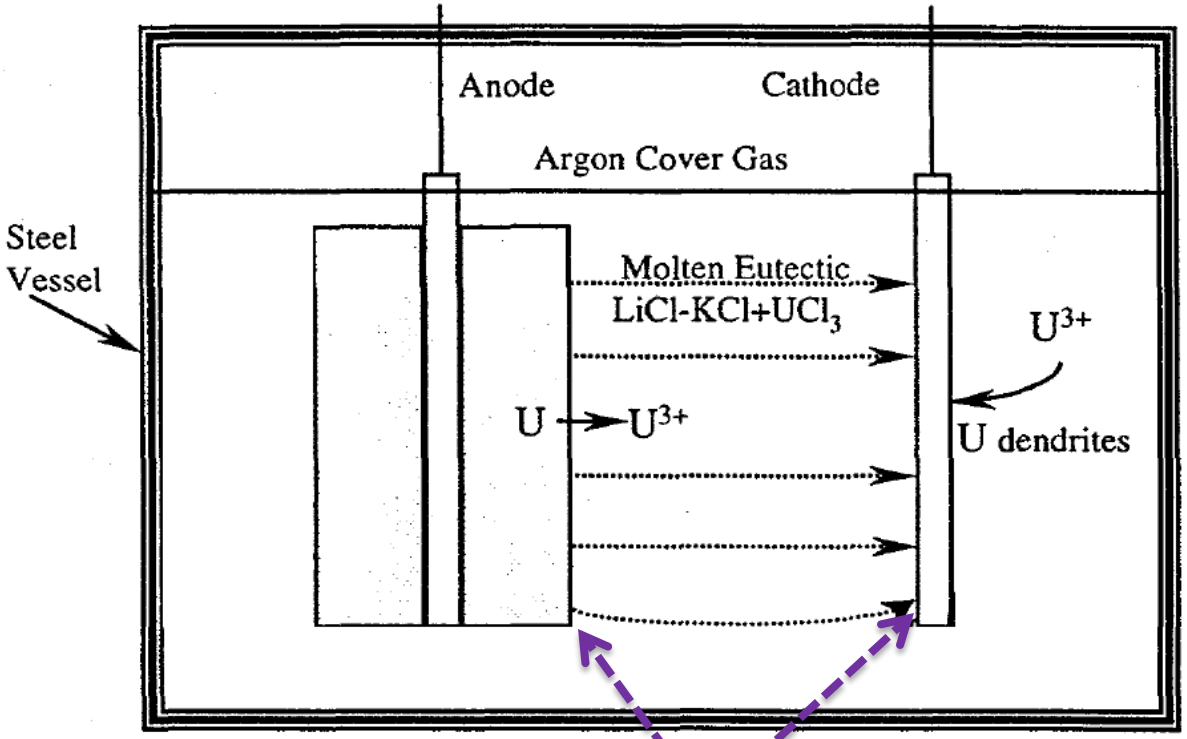


UNC INSTITUTE FOR THE ENVIRONMENT

Electro-Refiner Models

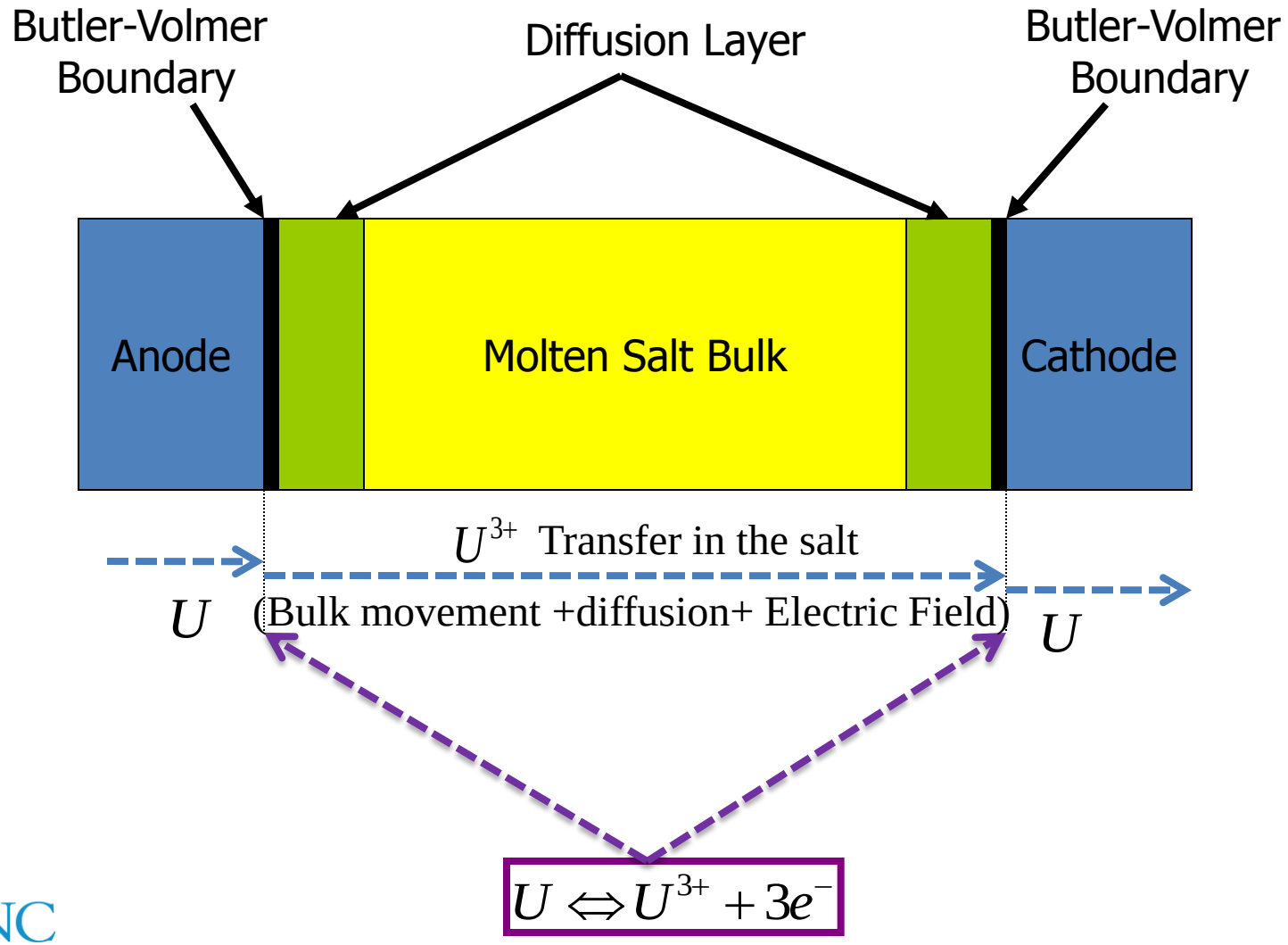
- ANL (PYRO, GPEC, Engineering model of Mk-V)
- INDIA (Numerical simulation)
- JAPAN (TRAIL, DEVON)
- INL/UI: 1D and 2D Model
- KAERI/SEOUL: REFIN + 3D Hydro-dynamic

Mark-IV Direct Deposit Mode



$$U \Leftrightarrow U^{3+} + 3e^{-}$$

Mass Transfer Process



Overview of CFD Model

- 3D Simulation of the Mark-IV Electro-Refiner
- Comprehensive modeling of the effect of fluid dynamic, electric field, electro-chemical reaction
- Reactions assumed to happen at the interface of molten salt and electrode/Cd pool
- ANSYS-CFX coupled with in-house Fortran Program

Model Highlights

- Molten Salt is modeled as incompressible viscous fluid mixed with uranium and the rest of the compositions
- Mass transfer rate of each species at the electrode surface: $$N_j = \frac{i_j}{z_j F}$$
- Electro-chemical reaction rate described by Butler-Volmer equation:
$$i_j = i_{0,j}\left[\exp\left(\frac{z_j \beta F}{RT}\eta\right) - \exp\left(-\frac{z_j (1-\beta) F}{RT}\eta\right)\right]$$
- Cell Potential: $$E_{cell} = \eta_a + \Phi_{ohm} + \eta_c$$

Model Parameters

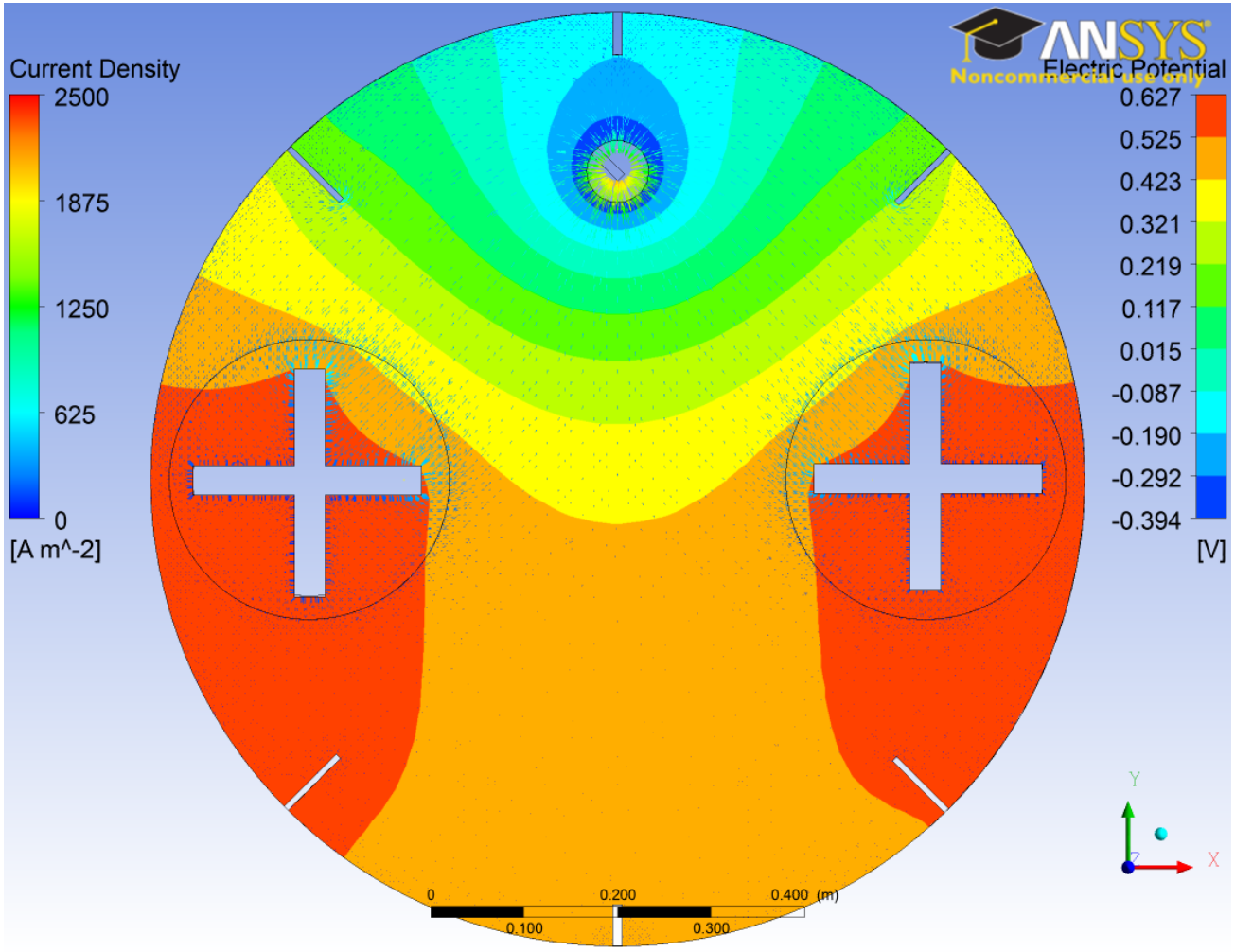
Species	U	Pu	Nd	Zr
Charge Number	3	3	3	4
Standard Electrode Potential (V vs. 1 wt% Ag/AgCl)	-1.249	-1.833	-2.358	-0.838
Diffusion Coefficient in Molten Salt (m2/s)	9.92E-10	1.08E-09	1.50E-09*	1.13E-09
Diffusion Coefficient in Cd (m2/s) *	1.50E-09	1.50E-09		
Activity Coefficient in Molten Salt	5.79E-03	6.62E-03	3.50E-03	4.48E-03
Activity Coefficient in Cd	7.50E+01	1.38E-04		
Exchange Current Density (A/m2)**	18	18	18	18
Transfer Coefficient*	0.5	0.5	0.5	0.5

* assumed value

** calculated value, assumed to be the same for all interfaces and species

The electric conductivity of the molten salt is 205 mho/m

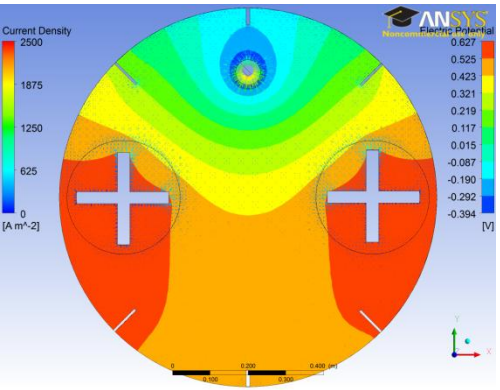
Current Density and Electric Potential (1)

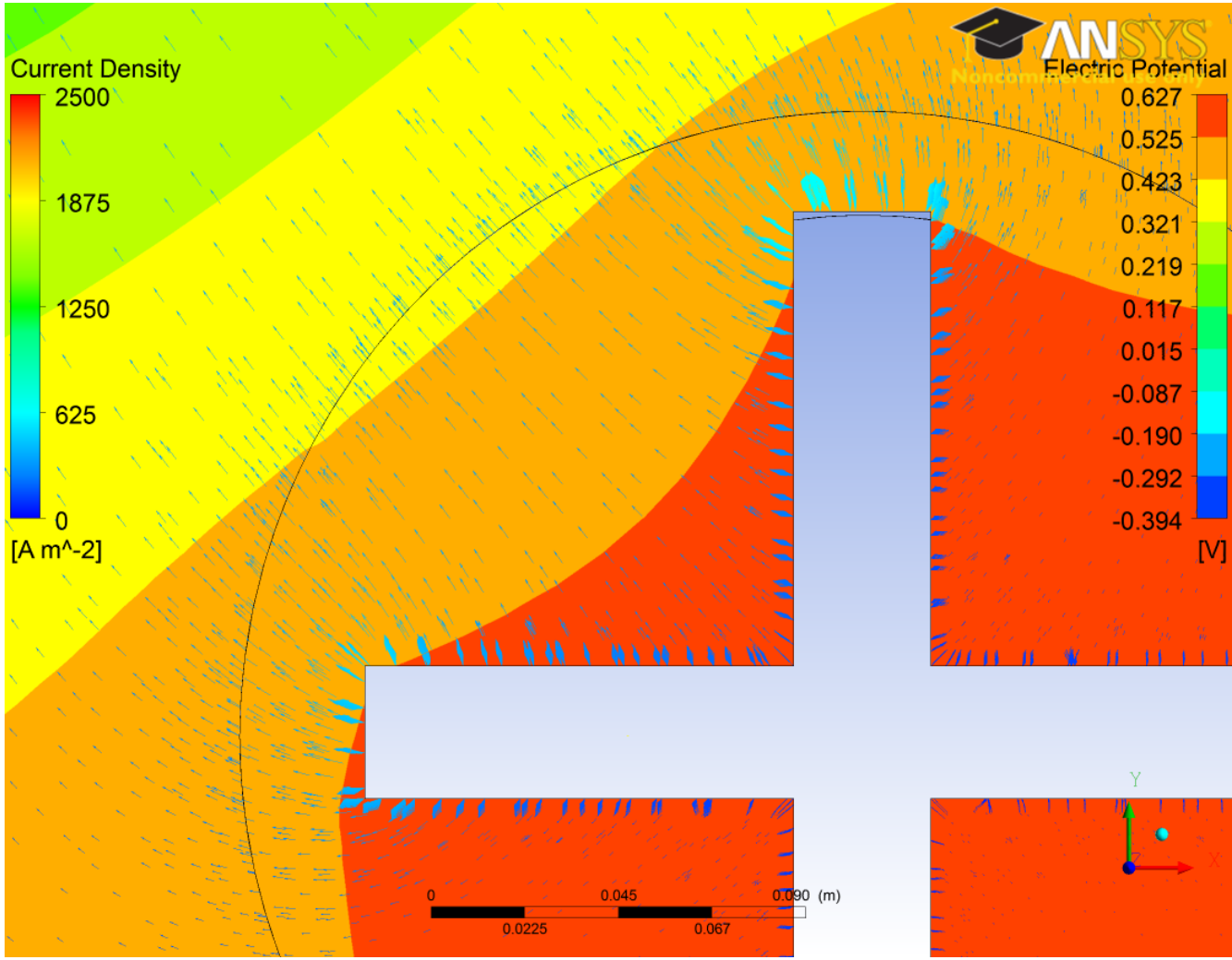


UNC INSTITUTE FOR THE ENVIRONMENT

Contour plot = Electric Potential Distribution
Vector plot = Current Density Distribution

Current Density and Electric Potential (2)

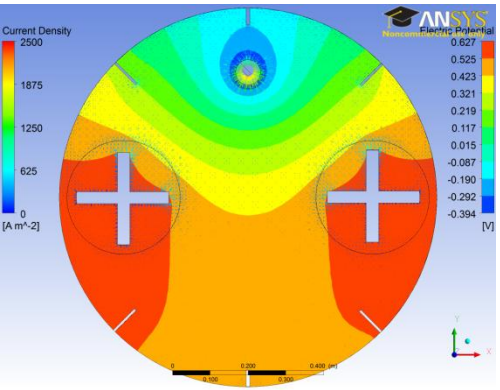


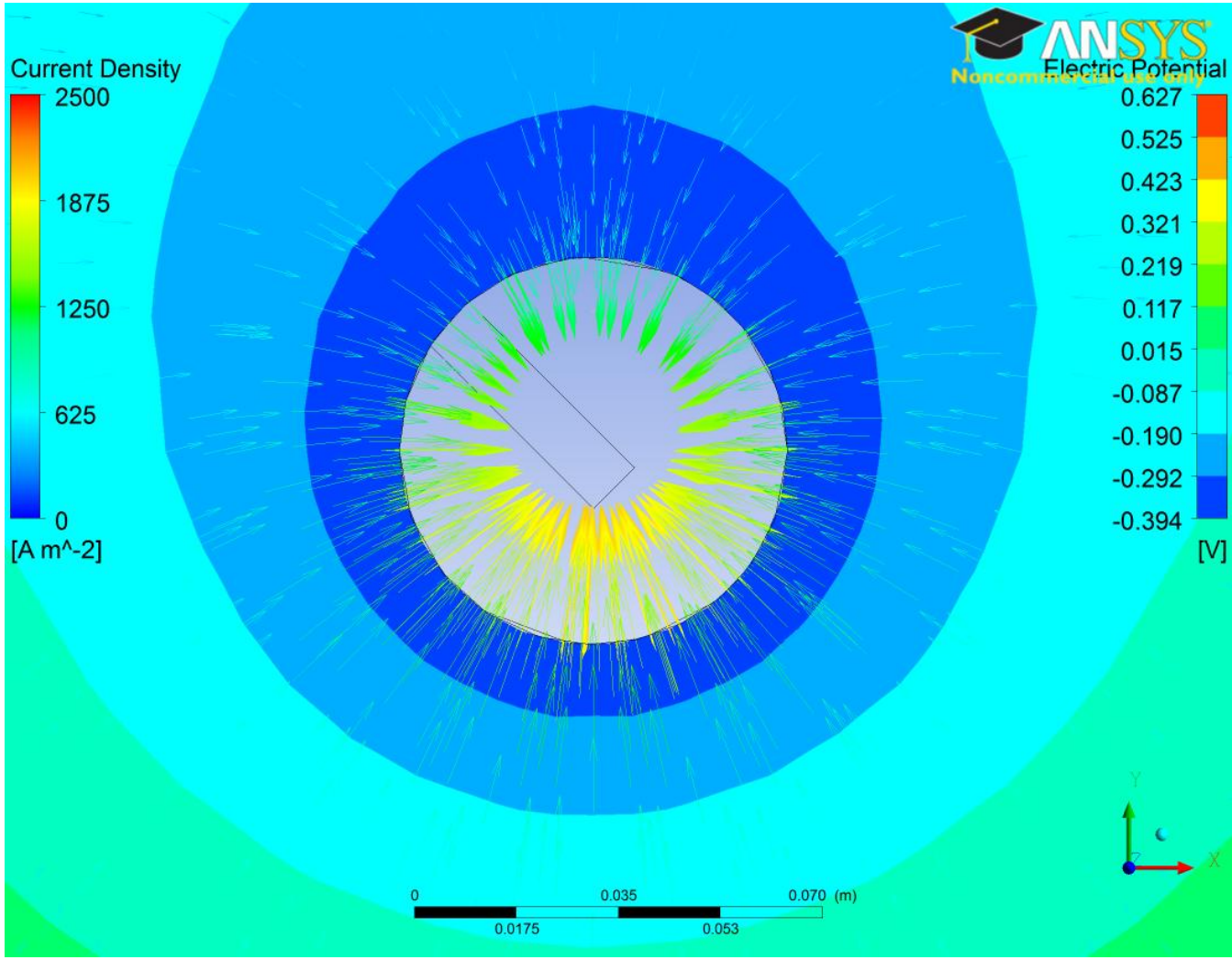


UNC INSTITUTE FOR THE ENVIRONMENT

Contour plot = Electric Potential Distribution
Vector plot = Current Density Distribution

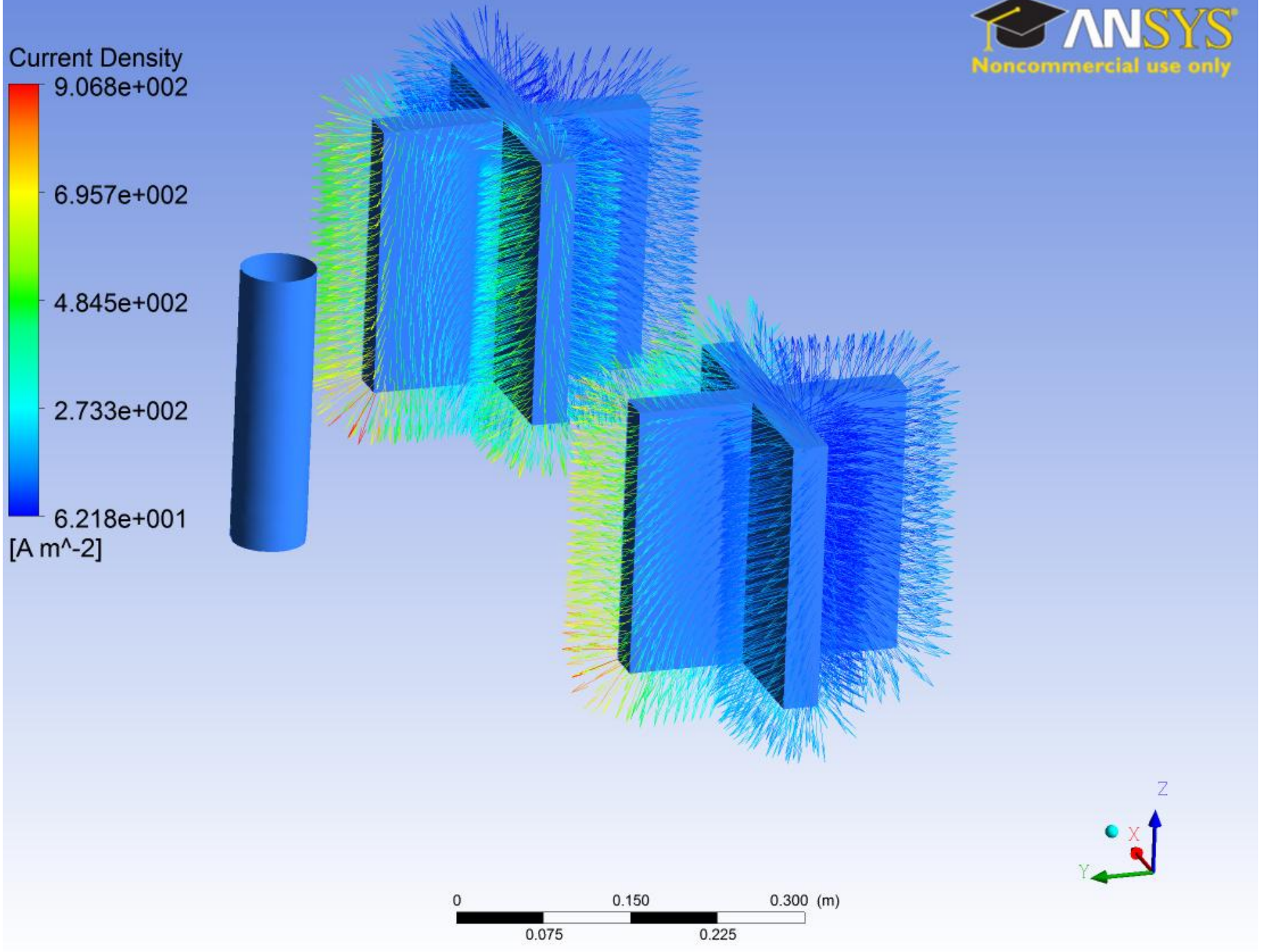
Current Density and Electric Potential (3)

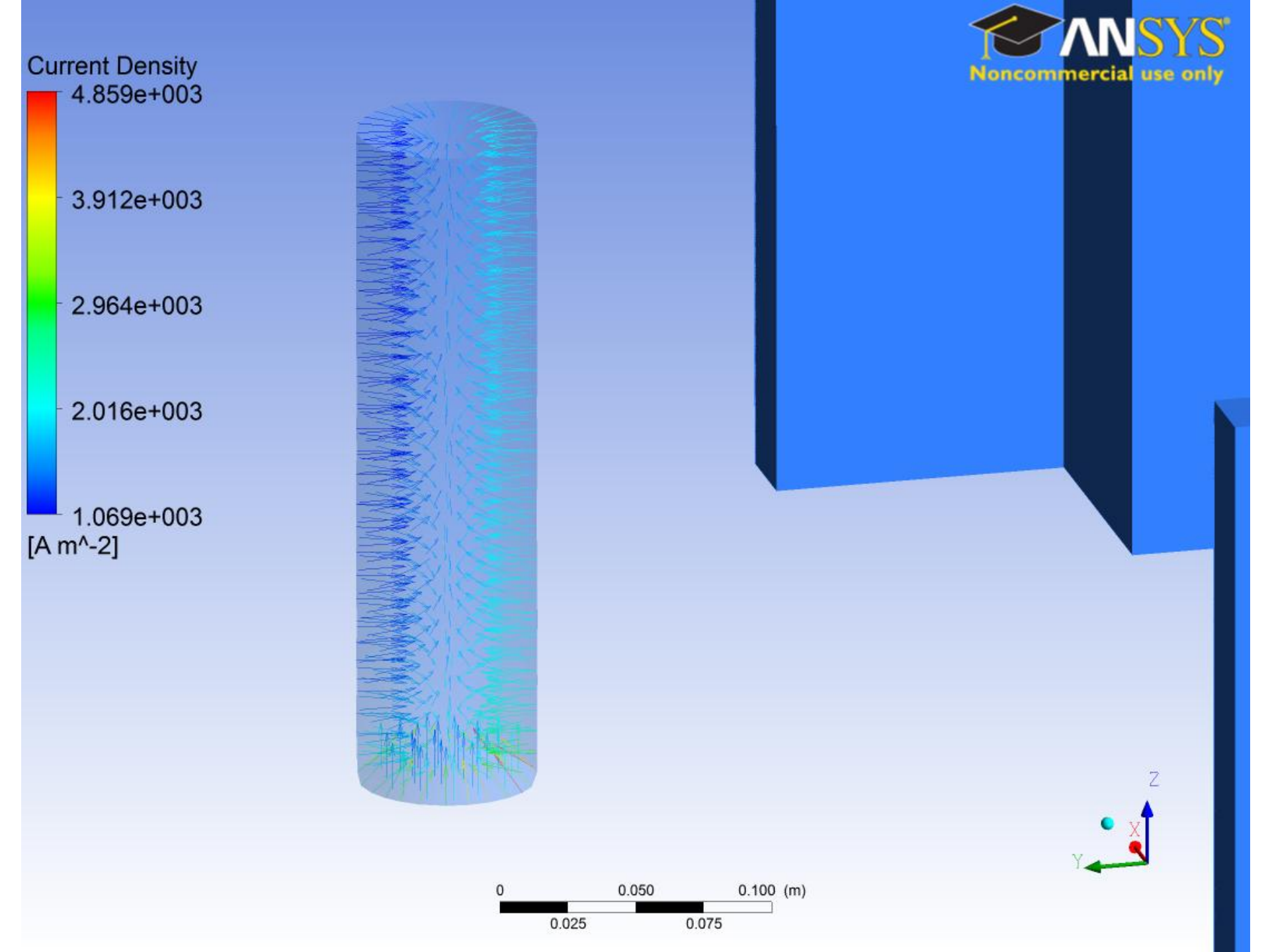




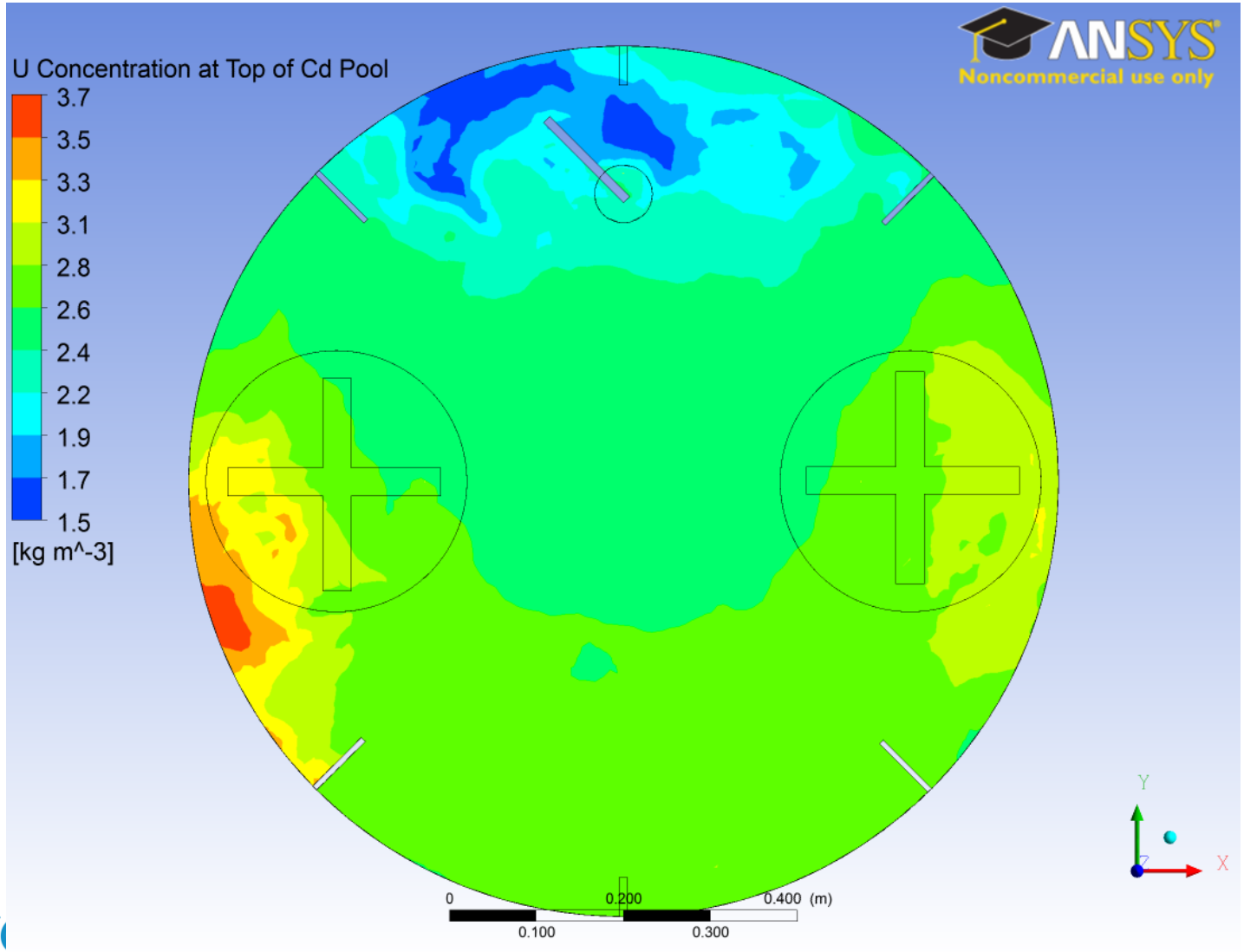
UNC INSTITUTE FOR THE ENVIRONMENT

Contour plot = Electric Potential Distribution
Vector plot = Current Density Distribution

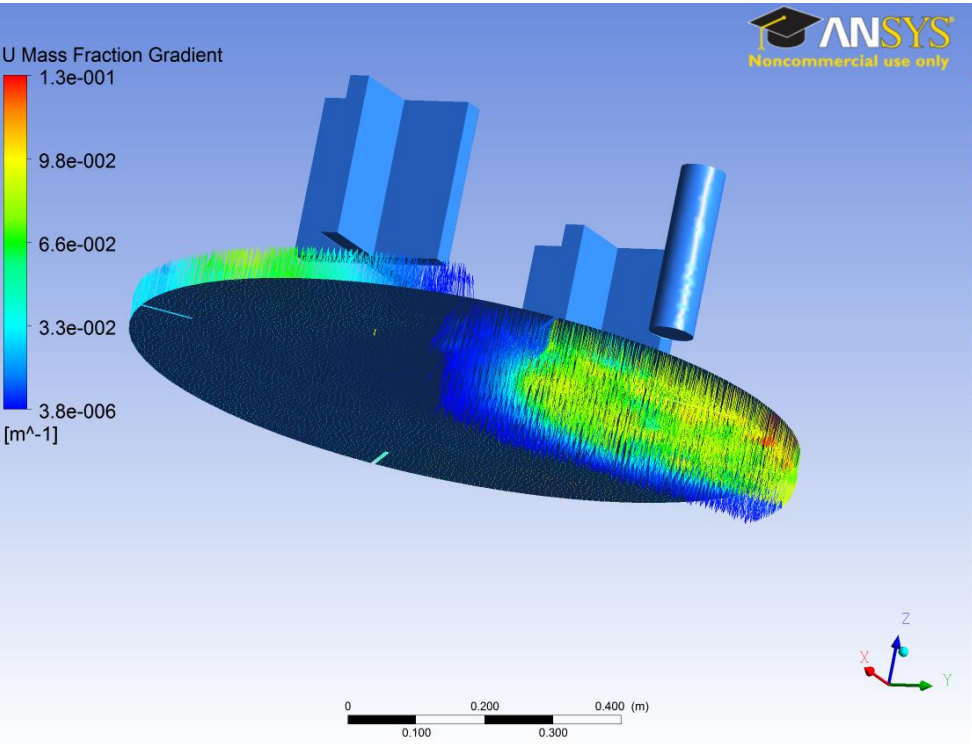

Current Density
9.068e+002
6.957e+002
4.845e+002
2.733e+002
6.218e+001
[A m^-2]
ANSYS
Noncommercial use only
Z
X
Y
0
0.150
0.300 (m)
0.075
0.225

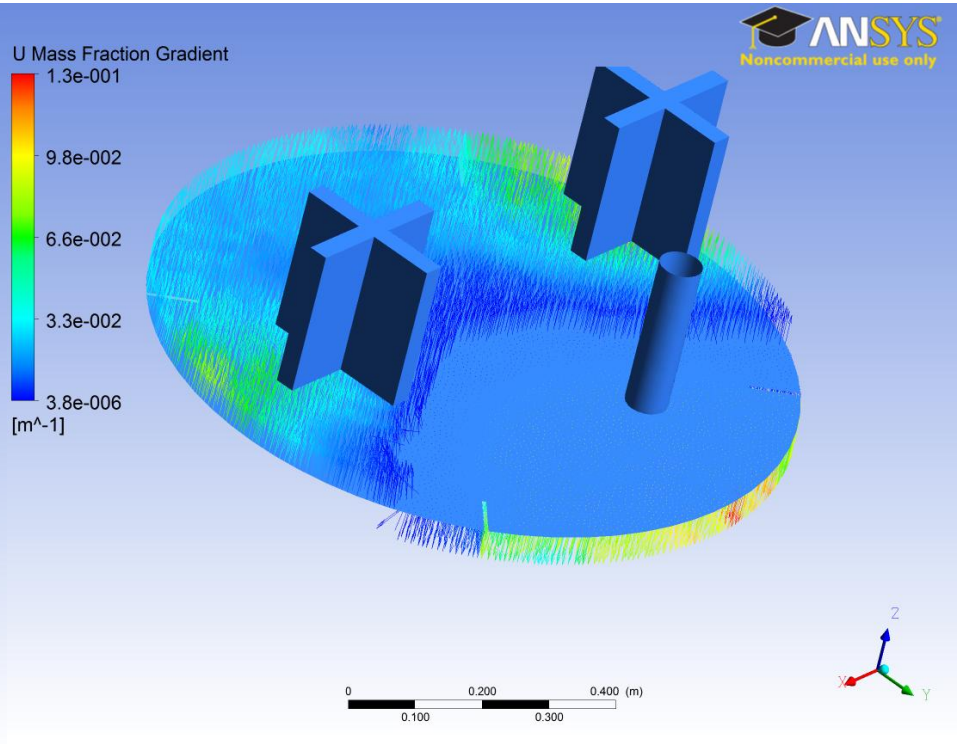

Current Density
4.859e+003
3.912e+003
2.964e+003
2.016e+003
1.069e+003
[A m^-2]
ANSYS
Noncommercial use only
Z
X
Y
0
0.050
0.100 (m)
0.025
0.075

U Concentration at Top of the Cd Pool

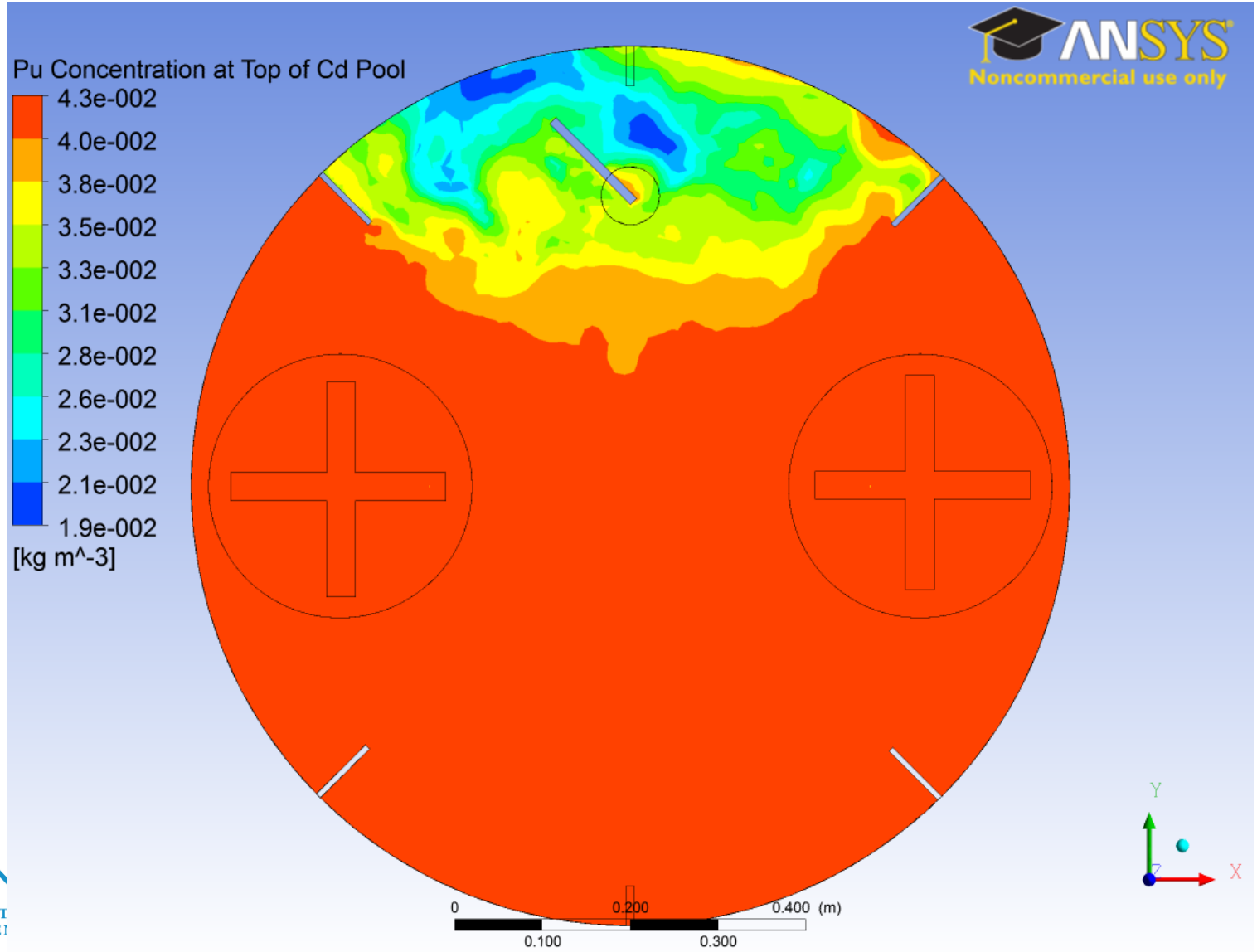


U Mass Fraction Gradient at Top of the Cd Pool

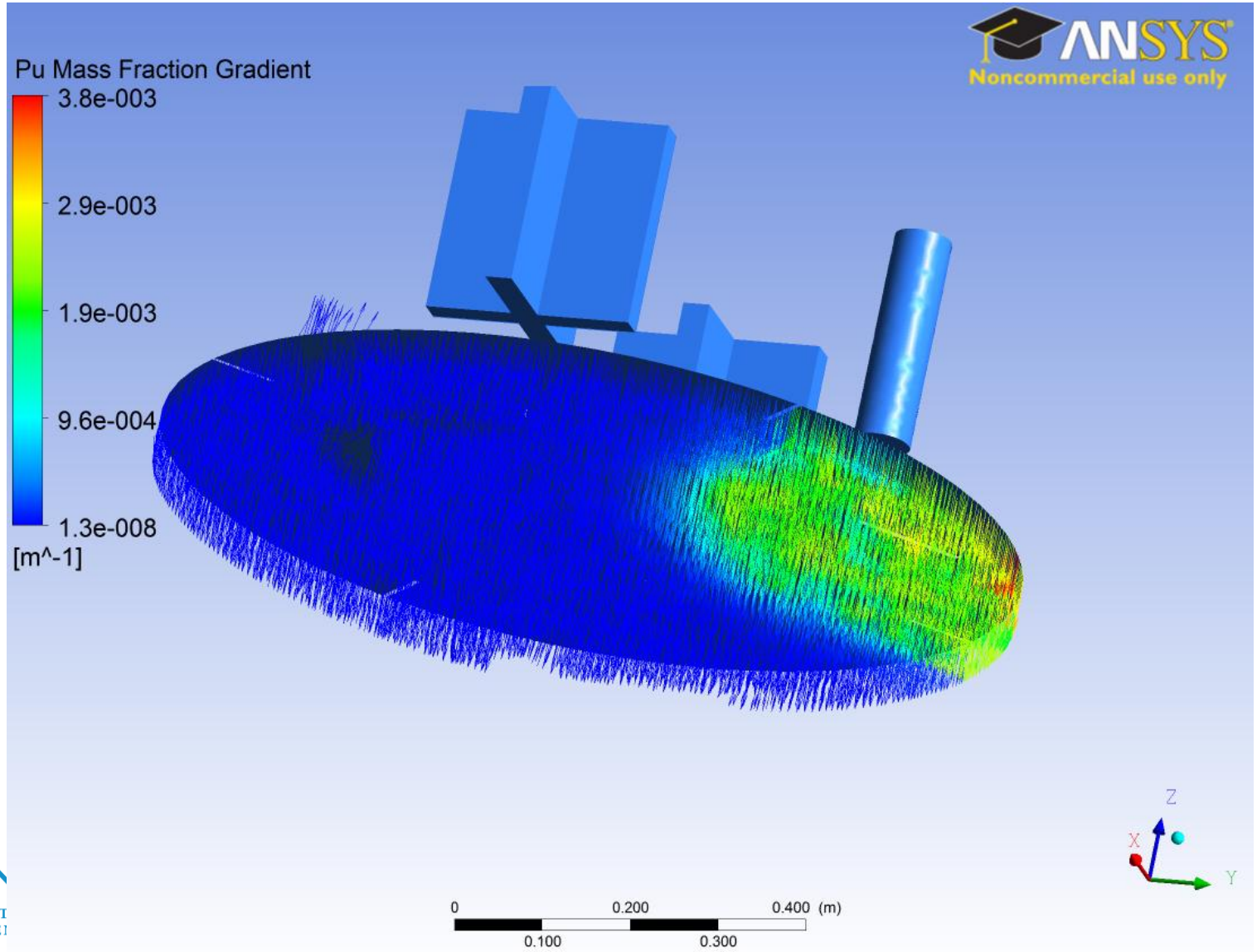




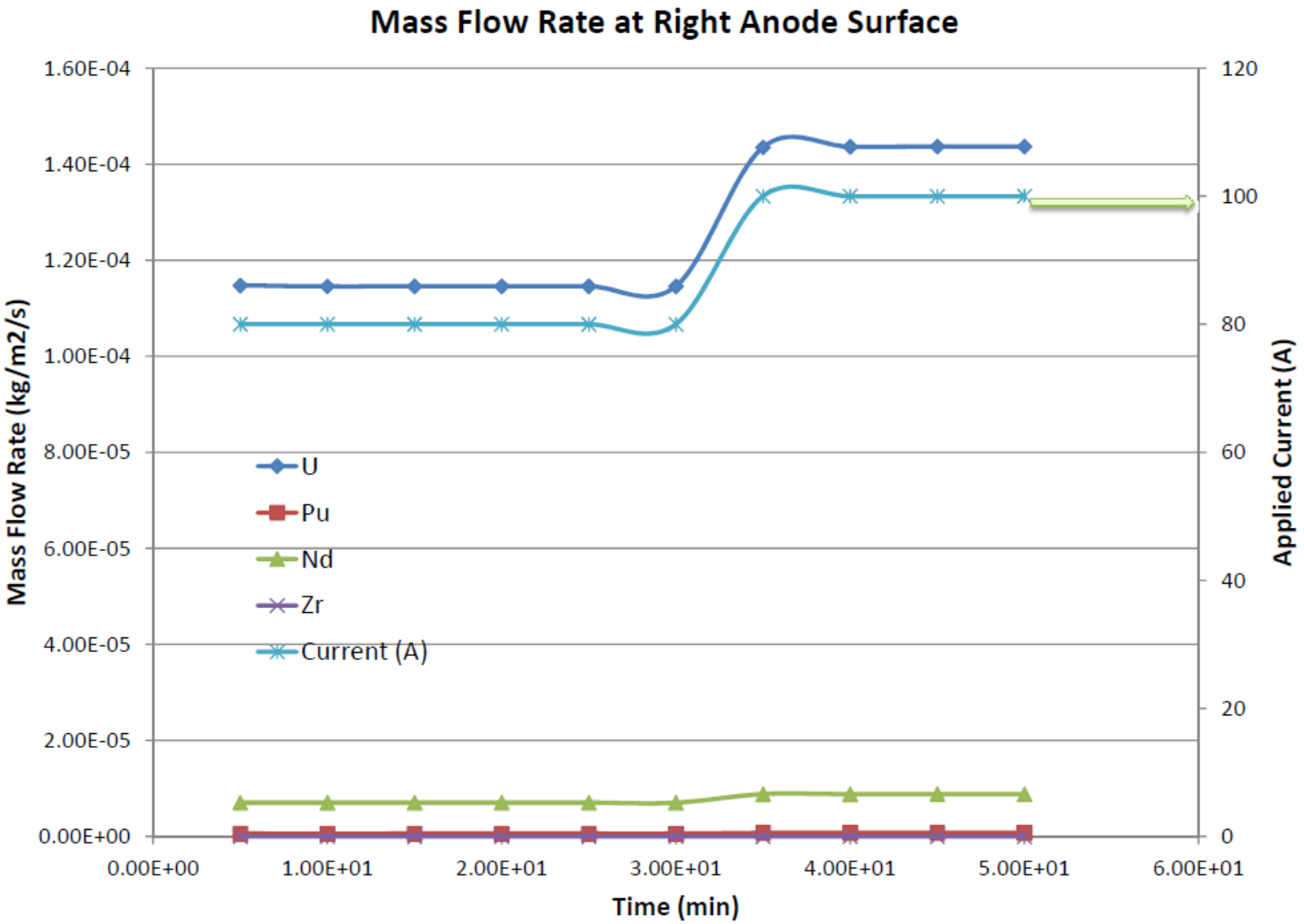
Pu Concentration at Top of the Cd Pool



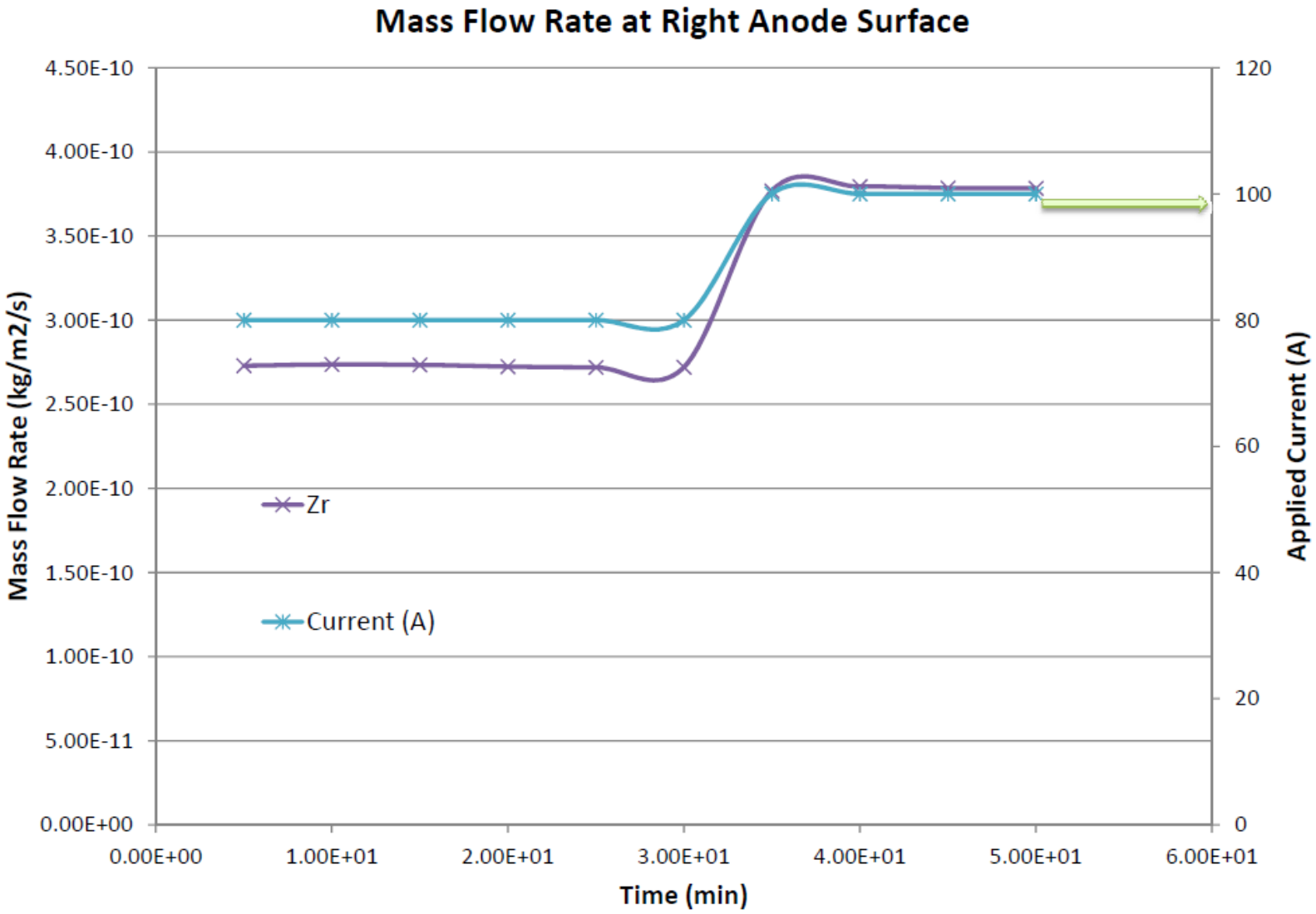
Pu Mass Fraction Gradient at Top of the Cd Pool



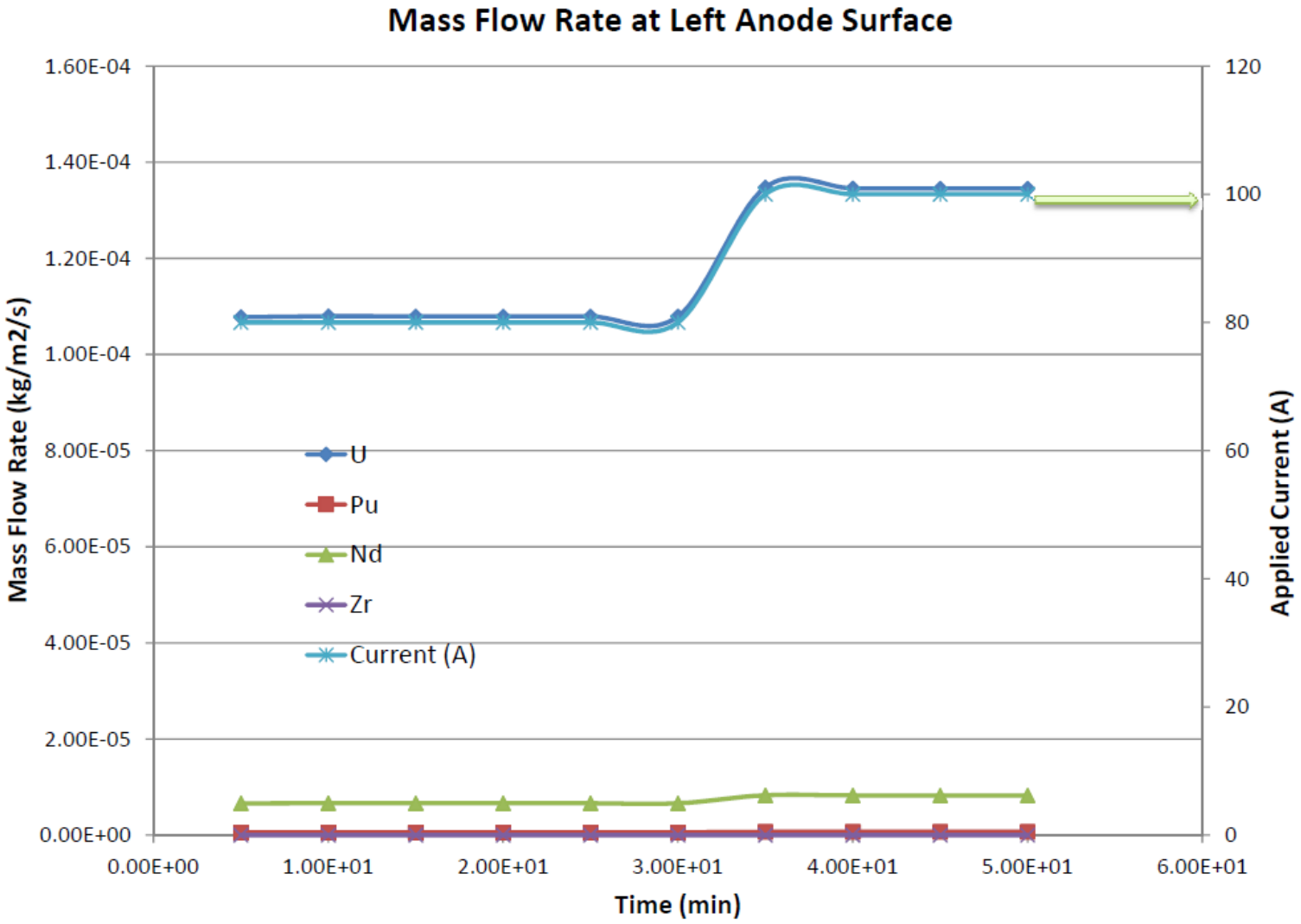
Mass Flow Rate at Anode (1)



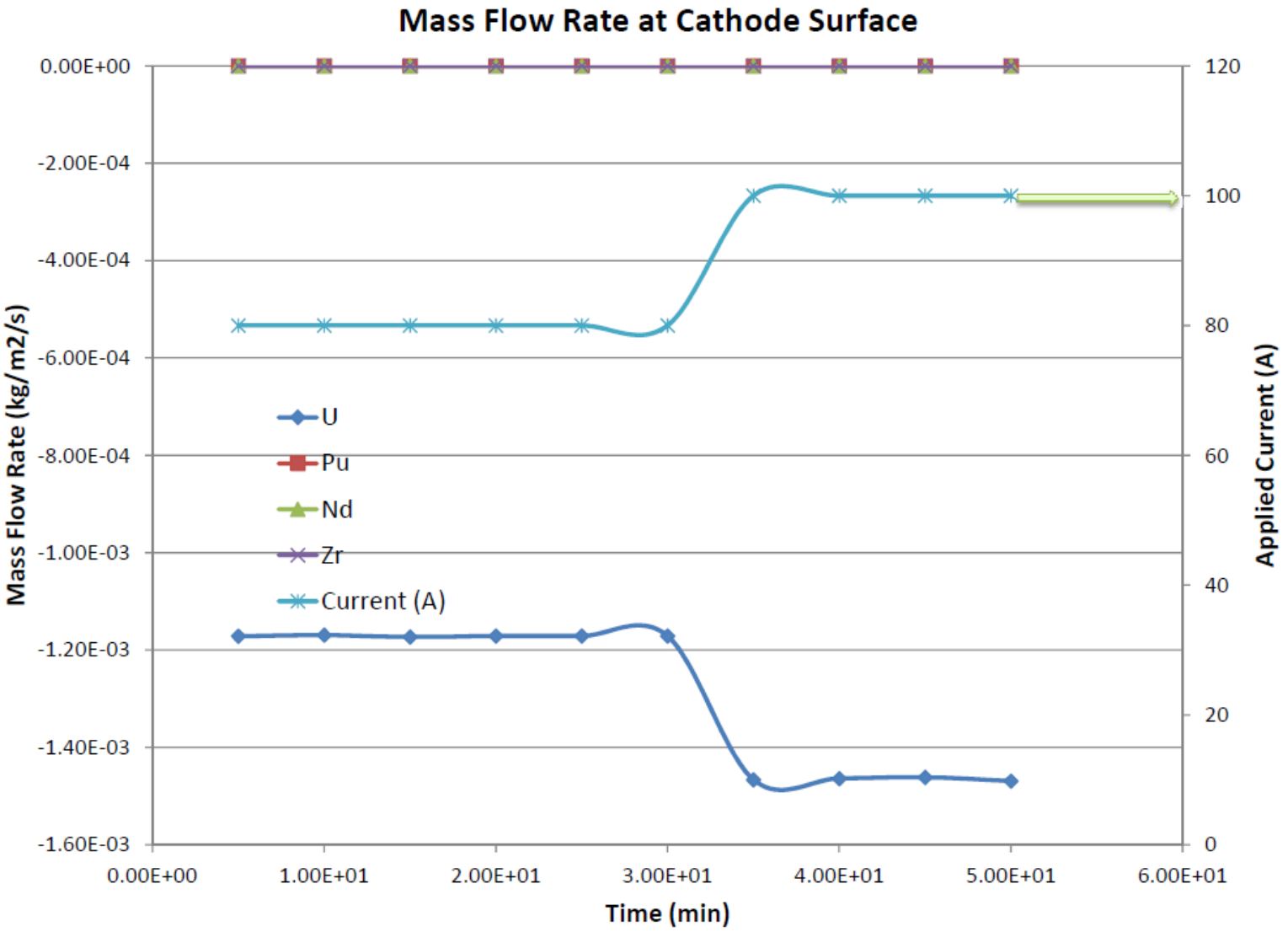
Mass Flow Rate at Anode (2)



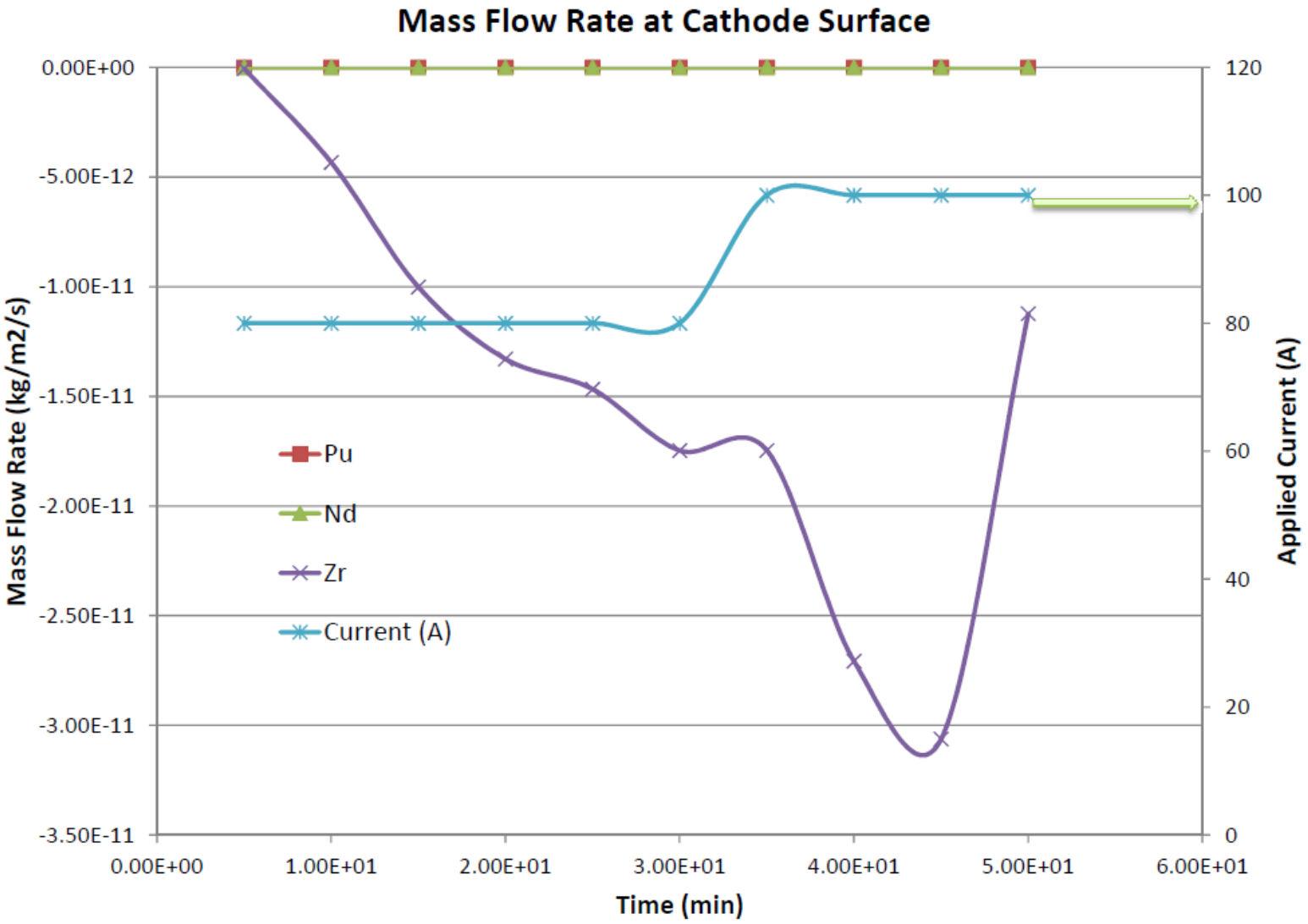
Mass Flow Rate at Anode (3)



Mass Flow Rate at Cathode (1)

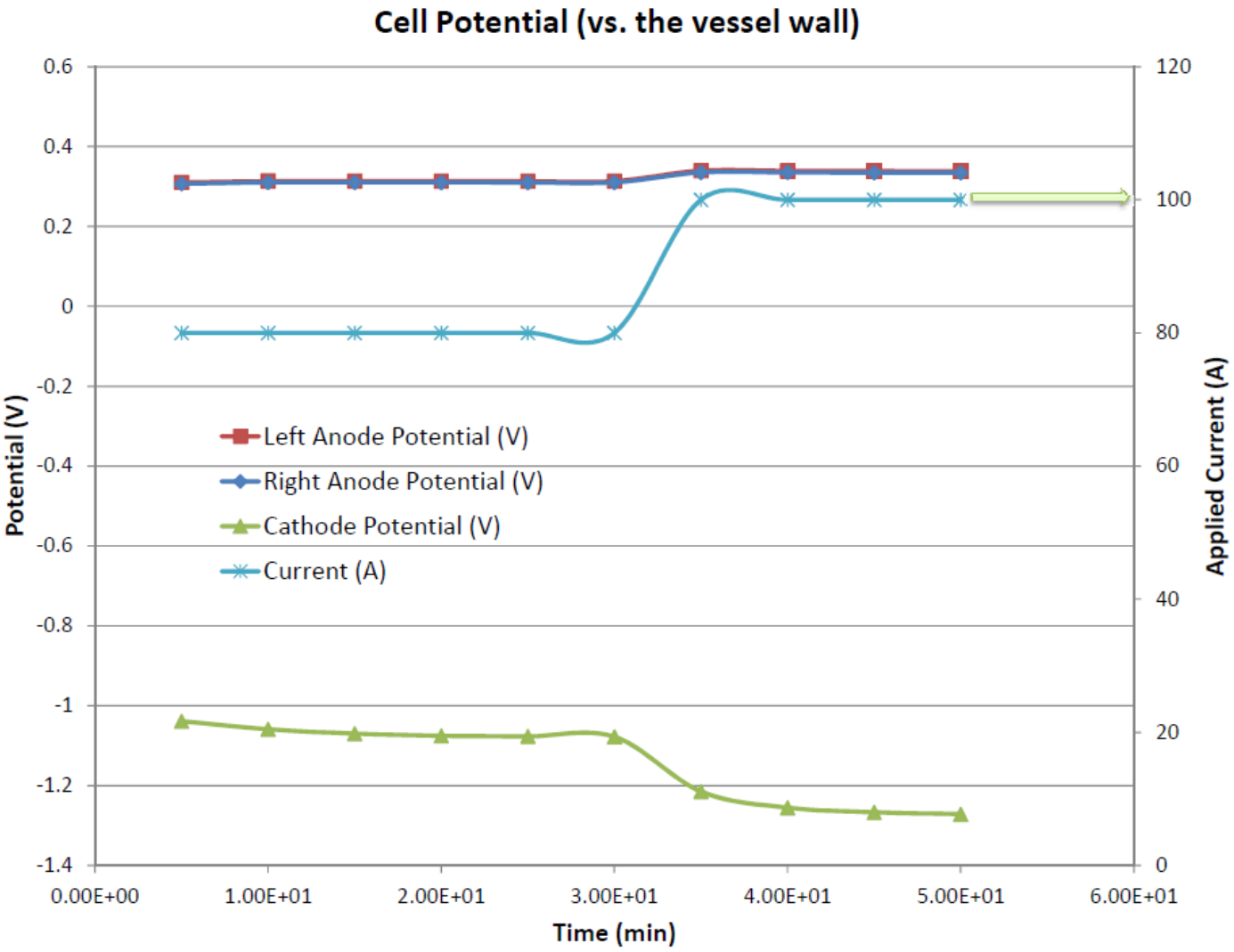


Mass Flow Rate at Cathode (2)



IN THE ENVIRONMENT

Cell Potentials



Observations

- Electric field distribution affects the electric-chemical reaction rate
- Zr is dissolving slowly during the direct deposit mode even when anode voltage is low
- Cd pool is serving as a “passing tunnel” for U
- Region in Cd pool closer to the anodes has higher concentration of U and Pu

Discussion

- Experimental data is needed to validate the model:
  - Model error
  - Parameter error
- Application of the model:
  - Determine parameters
  - Parameter sensitivity study – guide the experiments
  - Mass tracking/material accountability/safeguard