ALL CODES ARE IN FORTRAN 77

PROBLEM I

1. The codes were written with some non-dimensional variables different from those in paper. They are given below. Primes are used for these. Nomenclature for dimensional variables is same as in the paper. The different variables are:

$$\tau' = \frac{Dt}{L^2}, \Lambda' = \frac{|I|L}{DC_{ref}nF}$$

   Hence, these are related to those in the paper as follows:

$$\tau = \tau' \frac{D_1}{D}, \Lambda = \Lambda' \frac{D}{D_1}$$

2. Some are defined in the code only.

$$\text{kay\_1} = \kappa_1' = \kappa_1 \frac{D_1}{D}, \ \text{kay\_2} = \kappa_2' = \kappa_3 \frac{D_1}{D}$$

$$\text{cap\_gamma} = \frac{|I|L}{DnF}, \text{c\_not} = C_{ref}, \ \text{hence} \ \frac{\text{cap\_gamma}}{\text{c\_not}} = \Lambda'$$

   delta_tau = delta_τ' is the increment in time step.

3. Other variables in the code are same as in the paper: deltai=Δ_i,alambda(k)=λ_k, ai(k),bi(k) are the coefficients in the k^{th} eigenfunction.

Code named iteration_uniform_ic.f

This is the code to compute κ_1' and κ_3' as a function of τ'.
The input data are in these files:

1. input_plotcheq.dat contains geometry of the cell
2. output_normalized_vector.dat contains information on eigenvalues and normalized eigenfunction coefficients
3. inner_prod_uniform_ic_diff_5bc.dat contains data on the inner product of the uniform initial condition with the eigenfunctions.
4. operating.dat contains information for running program and also to change Λ' through cap_gamma.

The first three data files are common between problem I and III. They are placed in the directory code_problem_I to avoid unnecessary repetition. The output file is output_iteration_general.dat. Second column is τ'. The last two columns are kay_1 and kay_2. The middle columns are the second terms of

the r.h.s. in the second equation of eq.33 of the paper for each eigenfunction. This data is used The first term of the first equation of eq.33 of the paper is a linear decreasing function of time as seen from eq.33. Both these are used to construct concentration profile using the following code.

Code named conc_profile.f

This constructs concentration profile using eq.32 of the paper. The notation is same as described above and is a straight forward summation. output_conc_profile.dat is the output file. The output is u vs. ξ as different values of τ'.

All code files and data files are in the directory code_problem_I.

PROBLEM III

Many items and files are common to problem I. Hence, only differences will be mentioned here.

1. The new quantities defined make computation easier. These are udotz0(i) = $\langle \mathbf{u}.\mathbf{Z}_o \rangle (\tau')$ and udotz(i,j) = $\langle \mathbf{u}.\mathbf{Z}_j \rangle (\tau')$

2. cs1max and cs3max are $C_{s1,max}$ and $C_{s3,max}$ of paper.

3. u4 and u5 are u_4 and u_5 of paper.

Code named iteration_uniform_ic_non_linear.f

This is the code to compute κ_1', κ_3', and $u_i(\xi)$ as a function of τ'. conc_profile.f was integrated into iteration program in this code.

Only new input file is operating_non_linear.dat instead of operating.dat as it needs data on lithium concentration in the active materials.

The output files are

1. first three columns of output_iteration_general.dat are i (the time index), kay_1 and kay_2.

2. output_li_content.dat gives i (the time index) against u_4 and u_5 as a function of j (index of ξ).

3. output_conc_profile.dat gives i (the time index) versus u_1,u_2,u_3 as a function of j (index of ξ).

All code files and data files are in the directory code_problem_III.

PROBLEM II

1. The codes were written with some non-dimensional variables different from those in paper. They are given below. Primes are used for these.

Nomenclature for dimensional variables is same as in the paper. These are as follows:

$$\tau' = \frac{D_1 t}{L_1^2}, \Lambda' = \frac{|I| L_1}{D_1 C_{ref} n F}$$

Hence, these are related to those in the paper as follows:

$$\tau = \tau' \frac{L_1^2}{L^2}, \Lambda = \Lambda' \frac{L}{L_1}$$

2. Some are defined in the code only.

   $\text{alpha} = \frac{L_1}{L - L_1}$, beta(j) $= \lambda(j)$, cap_lambda $= \Lambda'$, akappa $= \kappa_1'$, u1 $= u_m$, conc(i) $= u_1(\xi)$

   $$\kappa_1' = \kappa_1 \frac{L_1^2}{L^2}$$

   g(i) $= g(\tau)$of eq.A.18, u_dot_z_zero(i) $= \langle \mathbf{u}.\mathbf{Z}_o \rangle (\tau)$, u_dot_zjxi(i) $= \sum_j \langle \mathbf{u}.\mathbf{Z}_j \rangle (\tau) Z_j(\xi)$

3. const_norm(j) are the normalization constants for eigenfunctions, eq.(A.12) of paper.

Code named program_iteration_v_4.f

This is the iteration program. It generates results for tau,i (index for time), u1(i), akappa(i), u_dot_z_zero(i) in the output file named output_plot_tau_u1.dat. The input files are

1. input_test_ev.dat for eigen values
2. input_iteration.dat for giving inputs including cap_lambda for changing operating conditions.

Code named program_conc_xi_v_2.f

Reads output from previous program and generates concentration profiles using eq.41 of paper. The output is in the file output_all_xi_tau.dat. It gives $u_1(\tau)$ at each value of ξ.

All code files and data files are in the directory code_program_II.