

*BATTERY

The keyword *BATTERY provides input data for the electrochemistry solver:

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*BATTERY_DATABASE_HISTORY_ALLNDS_ON_ELESET  
*BATTERY_DATABASE_HISTORY_GLOBALS  
*BATTERY_DATABASE_HISTORY_NODELIST_ON_ELESET  
*BATTERY_ECHEM_CELL_GEOMETRY  
*BATTERY_ECHEM_CONTROL_SOLVER  
*BATTERY_ECHEM_INITIAL  
*BATTERY_ECHEM_MAT_ANODE  
*BATTERY_ECHEM_MAT_CATHODE  
*BATTERY_ECHEM_MAT_ELECTROLYTE  
*BATTERY_ECHEM_THERMAL
```

For now, the available capability involves a one-dimensional electrochemistry solver that is coupled to the structural mechanics and structural thermal solver in each structural element identified as being part of a battery cell.

BATTERY**BATTERY_DATABASE_HISTORY_ALLNDS_ON_ELESET*****BATTERY_DATABASE_HISTORY_ALLNDS_ON_ELESET**

Purpose: Enable output of battery electrochemistry solver data for all one-dimensional battery mesh nodes on each element in an element set. The output goes to binary database binout.

Card 1	1	2	3	4	5	6	7	8
Variable	DT	LCUR	IOOPT	ESID				
Type	F	I	I	I				
Default	0.0	0	0	none				

VARIABLE	DESCRIPTION
DT	Time interval between outputs. If DT is zero, no output is generated.
LCUR	Optional curve ID specifying the time interval between outputs. Use *DEFINE_CURVE to define the curve; the abscissa is time, and the ordinate is time interval between outputs.
IOOPT	Flag to govern behavior of the output frequency load curve defined by LCUR: EQ.1: When output is generated at time t_n , the next output time t_{n+1} is computed as $t_{n+1} = t_n + \text{LCUR}(t_n)$. This is the default behavior. EQ.2: When output is generated at time t_n , the next output time t_{n+1} is computed as $t_{n+1} = t_n + \text{LCUR}(t_{n+1})$. EQ.3: Output is generated for each abscissa point in the load curve definition. The actual value of the load curve is ignored.
ESID	ID of a *SET_SOLID element set to use for the binout operation. The selected elements in the element set of volume structural elements must also be battery electrochemistry elements.

BATTERY_DATABASE_HISTORY_NODELIST_ON_ELESET**BATTERY*****BATTERY_DATABASE_HISTORY_NODELIST_ON_ELESET**

Purpose: Enable output of battery electrochemistry solver data for a specified set of one-dimensional battery mesh nodes on each element in an element set. The output goes to binary database binout.

Card 1	1	2	3	4	5	6	7	8
Variable	DT	LCUR	IOOPT	ESID				
Type	F	I	I	I				
Default	0.0	0	0	none				

Node ID Cards. Battery mesh nodes to select for battery data output in the elements selected by ESID in Card 1. Include as many cards as needed. This input ends at the next keyword ("**") card.

Card 2	1	2	3	4	5	6	7	8
Variable	NID1	NID2	NID3	NID4	NID5	NID6	NID7	NID8
Type	I	I	I	I	I	I	I	I

VARIABLE	DESCRIPTION
DT	Time interval between outputs. If DT is zero, no output is generated.
LCUR	Optional curve ID specifying the time interval between outputs. Use *DEFINE_CURVE to define the curve; the abscissa is time, and the ordinate is time interval between outputs.
IOOPT	Flag to govern behavior of the output frequency load curve defined by LCUR: EQ.1: When output is generated at time t_n , the next output time t_{n+1} is computed as $t_{n+1} = t_n + \text{LCUR}(t_n).$ This is the default behavior.

BATTERY**BATTERY_DATABASE_HISTORY_NODELIST_ON_ELESET**

VARIABLE	DESCRIPTION
	EQ.2: When output is generated at time t_n , the next output time t_{n+1} is computed as $t_{n+1} = t_n + \text{LCUR}(t_{n+1}).$
	EQ.3: Output is generated for each abscissa point in the load curve definition. The actual value of the load curve is ignored.
ESID	ID of a *SET_SOLID element set to use for the binout operation. The selected elements in the element set of volume structural elements must also be battery electrochemistry elements.
NID <i>i</i>	Node ID <i>i</i>

***BATTERY_DATABASE_HISTORY_GLOBALS**

Purpose: Enable output of battery electrochemistry solver data. The output goes to binary database binout.

Card 1	1	2	3	4	5	6	7	8
Variable	DT	LCUR	IOOPT					
Type	F	I	I					
Default	0.0	0	0					

VARIABLE	DESCRIPTION
DT	Time interval between outputs. If DT is zero, no output is generated.
LCUR	Optional curve ID specifying the time interval between outputs. Use *DEFINE_CURVE to define the curve; the abscissa is time, and the ordinate is time interval between outputs.
IOOPT	Flag to govern behavior of the output frequency load curve defined by LCUR: EQ.1: When output is generated at time t_n , the next output time t_{n+1} is computed as $t_{n+1} = t_n + \text{LCUR}(t_n)$. This is the default behavior. EQ.2: When output is generated at time t_n , the next output time t_{n+1} is computed as $t_{n+1} = t_n + \text{LCUR}(t_{n+1})$. EQ.3: Output is generated for each abscissa point in the load curve definition. The actual value of the load curve is ignored.

*BATTERY

*BATTERY_ECHEM_CELL_GEOMETRY

*BATTERY_ECHEM_CELL_GEOMETRY

Purpose: Set general-purpose geometry variables for a single cell BATTERY model.

Card 1	1	2	3	4	5	6	7	8
Variable	IMODEL	ALEN	SLEN	CLEN	ACCLEN	CCCLEN		
Type	I	F	F	F	F	F		
Default	none	none	none	none	none	none		

Card 2	1	2	3	4	5	6	7	8
Variable	NELEA	NELES	NELEC	NELECCA	NELECCC			
Type	I	I	I	I	I			
Default	none	none	none	none	none			

VARIABLE	DESCRIPTION
IMODEL	Battery model identifier (see Remark 1)
ALEN	Length of the anode side electrode
SLEN	Length of the separator
CLEN	Length of the cathode side electrode
ACCLEN	Length of the negative current collector
CCCLEN	Length of the positive current collector
NELEA	Number of elements in the anode electrode
NELES	Number of elements in the separator
NELEC	Number of elements in the cathode electrode
NELECCA	Number of elements in the anode current collector

VARIABLE	DESCRIPTION
NELECCC	Number of elements in the cathode current collector

Remarks:

1. **Identifier.** The battery model identifier (IMODEL) should match the IMODEL value specified in the corresponding *BATTERY_ECHEM_CONTROL_SOLVER card. If a different value is given, the value on the *BATTERY_ECHEM_CONTROL_SOLVER card will be the default.

*BATTERY

*BATTERY_ECHEM_CONTROL_SOLVER

*BATTERY_ECHEM_CONTROL_SOLVER

Purpose: Set general purpose control variables for a battery electrochemistry simulation.

Card Summary:

Card 1. This card is required.

IMODEL	IDIMEN	NCYCLE	IAGING	ITRA	IGAS		
--------	--------	--------	--------	------	------	--	--

Card 2. Include NCYCLE instances of this card, one for each cycle.

CMODE	CTYPE	CEND	TCUT	VCUT	RCURR		
-------	-------	------	------	------	-------	--	--

Card 3.1. Include this card if IAGING = 1.

SEIMW	SEIRHO	SEIBRUG	SEIEPS	SEICO	SEITO		
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Card 3.2. Include this card if IAGING = 1.

SEIIO	SEIRKA	SEICON	ECCO	ECDFS			
-------	--------	--------	------	-------	--	--	--

Card 4.1. Include this card if ITRA = 1.

AFI	EAT	HOFEC	HOFLI	HOFLED			
-----	-----	-------	-------	--------	--	--	--

Card 4.2. Include this card if ITRA = 1.

HOFC2H4	HOFLC	HOFC02	HOF02				
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Card 5. Include this card if IGAS = 1.

IC2H4	I02	IC02	IH20	AG1	AG2	EG1	EG2
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Data Card Definitions:

Card 1	1	2	3	4	5	6	7	8
Variable	IMODEL	IDIMEN	NCYCLE	IAGING	ITRA	IGAS		
Type	I	I	I	I	I	I		
Default	none	none	1	1	0	0		

VARIABLE	DESCRIPTION
IMODEL	Sets the battery model: EQ.1: Dual insertion model (Newman). IAGING, ITRA, and IGAS must be set to 0. EQ.2: Multiphysics LIB model. With IGAS = 0, the model includes thermal effects while with IGAS = 1, the model includes both thermal and chemistry effects. Note that IAGING and ITRA must be set to 1 for either case. See Remark 1 . EQ.3: Lithium metal battery
IDIMEN	Sets the geometric dimension: EQ.1: 1D LIB models EQ.101: 1D models with thermo-mechanical coupling (available for IMODEL = 1 and 2). See Remark 2 .
NCYCLE	Number of cycles to run. Default is 1 cycle.
IAGING	Aging model flag (see Remark 3): EQ.0: Off EQ.1: On
ITRA	Thermal runaway model flag (see Remark 3): EQ.0: Off EQ.1: On
IGAS	Gas generation model flag (see Remark 4): EQ.0: Off EQ.1: On

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*BATTERY_ECHEM_CONTROL_SOLVER

Cycle Card. Include NCYCLE instances of this card, that is, one for each cycle.

Card 2	1	2	3	4	5	6	7	8
Variable	CMODE	CTYPE	CEND	TCUT	VCUT	RCURR		
Type	I	I	I	F	F	F		
Default	1	0	none	none	none	none		

VARIABLE	DESCRIPTION
CMODE	Battery running mode flag: EQ.0: Galvanostatic run EQ.1: Potentiostatic run (This is under development and not recommended.)
CTYPE	Running current type: EQ.0: Constant current EQ.1: Variable current
CEND	Cause of battery cycle termination: EQ.1: Cycle run for a given time period. EQ.2: Cycle run until a given cut-off voltage.
TCUT	Total running time for the cycle
VCUT	Cut-off voltage for the cycle
RCURR	Cycle operating current in the case of constant current

Aging Card 1. Include this card if IAGING = 1.

Card 3.1	1	2	3	4	5	6	7	8
Variable	SEIMW	SEIRHO	SEIBRUG	SEIEPS	SEICO	SEITO		
Type	F	F	F	F	F	F		
Default	0.0	0.0	0.0	0.0	0.0	0.0		

Aging Card 2. Include this card if IAGING = 1.

Card 3.2	1	2	3	4	5	6	7	8
Variable	SEII0	SEIRKA	SEICON	ECC0	ECDFS			
Type	F	F	F	F	F			
Default	0.0	0.0	0.0	0.0	0.0			

VARIABLE	DESCRIPTION
SEIMW	Molecular weight of the SEI
SEIRHO	Density of the SEI
SEIBRUG	The Bruggeman constant of the SEI
SEIEPS	Initial SEI porosity
SEICO	Initial SEI concentration (units: mol/m ³)
SEITO	Initial thickness of the SEI layer (units: m)
SEII0	Exchange current density for the SEI reaction
SEIRKA	Reaction rate constant for the SEI reaction (ignored if SEII0 ≠ 0.0)
SEICON	Ionic conductivity (units: S/m)
ECC0	Initial concentration of EC (ethylene carbonate). This field is ignored if SEII0 ≠ 0.0.

BATTERY**BATTERY_ECHEM_CONTROL_SOLVER**

VARIABLE	DESCRIPTION							
ECDFDS	Diffusion coefficient of EC							

Thermal Runaway Card 1. Include this card if ITRA = 1.

Card 4.1	1	2	3	4	5	6	7	8
Variable	AFI	EAT	HOFEC	HOFLI	HOFLED			
Type	F	F	F	F	F			
Default	0.0	0.0	0.0	0.0	0.0			

Thermal Runaway Card 2. Include this card if ITRA = 1.

Card 4.2	1	2	3	4	5	6	7	8
Variable	HOFC2H4	HOFLC	HOFCO2	HOFO2				
Type	F	F	F	F				
Default	0.0	0.0	0.0	0.0				

VARIABLE	DESCRIPTION
AFI	Frequency factor for the reaction
EAT	Activation energy for the reaction
HOFEC	Formation enthalpy of the EC (units: kJ/mol)
HOFLI	Formation enthalpy of the LI
HOFLED	Formation enthalpy of the SEI layer (units: kJ/mol)
HOFC2H4	Formation enthalpy of ethylene (units: kJ/mol)
HOFLC	Formation enthalpy of LC (Li_2CO_3 ; units: kJ/mol)
HOFCO2	Formation enthalpy of CO_2 (units: kJ/mol)
HOFO2	Formation enthalpy of O_2 (units: kJ/mol)

Gas Initial Conditions Card. Include this card if IGAS = 1.

Card 5	1	2	3	4	5	6	7	8
Variable	IC2H4	IO2	ICO2	IH2O	AG1	AG2	EG1	EG2
Type	F	F	F	F	F	F	F	F
Default	0.0	0.0	0.0	0.0	3.426E26	5.028E-6	2.50e5	2.51e5
Remarks					5	5	5	5

VARIABLE	DESCRIPTION
IC2H4	Initial concentration of C ₂ H ₂ gas (units: mol/m ³)
IO2	Initial concentration of O ₂ gas (units: mol/m ³)
ICO2	Initial concentration of CO ₂ gas (units: mol/m ³)
IH2O	Initial concentration of H ₂ O gas (units: mol/m ³)
AG1	Frequency factor for Ethylene oxidation (units: m/s)
AG2	Frequency factor for Lithium hydration (units: m/s)
EG1	Activation energy of Ethylene oxidation (units: J/mol)
EG2	Activation energy of Lithium hydration (units: J/mol)

Remarks:

- Multiphysics Battery Models.** With IMODEL = 2, you can model a battery with thermal effects or a battery with both thermal and chemistry effects depending on the value of IGAS. These two battery models include battery aging, thermal runaway, and battery swelling. The battery and chemistry effects model additionally includes a gas generation model for modeling the chemistry effects.
- Shutdown Key.** For coupled battery models (IDIMEN = 101) with IMODEL = 1 or 2, the shutdown key will work if the minimum ignition energy in the battery system reaches the critical condition like pre-thermal-runaway.
- Input Requirements for Aging and Thermal Runaway Models.** When IAGING = 1, all the variables on Cards 3.1 and 3.2 must be filled. A similar

requirement applies when ITRA = 1 in that all the variables of Cards 41 and 4.2 must be filled. For more details about these models, please see the Theory manual.

4. **Battery Chemistry Files.** When IGAS = 1, *CHEMISTRY_BATTERY must be included in the input deck to provide the file names for the battery chemistry input file, the corresponding thermodynamics data file, and the transport properties file. Please refer to the *CHEMISTRY chapter for further details about the *CHEMISTRY_BATTERY keyword.
5. **AG1, AG2, EG1, and EG2.** AG1, AG2, EG1, and EG2 are used to compute the rate of reaction based on Arrhenius equation as

$$r = A_k c_k e^{-\frac{EG_k}{RT}} .$$

A_k is the frequency factor for the reaction, c_k is the concentration, EG_k is the activation energy for the reaction, R is the universal gas constant, and T is the temperature.

BATTERY_ECHEM_INITIAL**BATTERY*****BATTERY_ECHEM_INITIAL**

Purpose: Initializes the composite electrodes and electrolyte in every element of the BATTERY simulation mesh.

Card 1	1	2	3	4	5	6	7	8
Variable	DT0	LICE	PHI1	LICS	CURRIC	FLUXIC	PHI2	
Type	F	F	F	F	F	F	F	
Default	none	none	none	none	none	none	none	

VARIABLE	DESCRIPTION
DT0	Initial time step size
LICE	Initial concentration of lithium ions in the electrolyte
PHI1	Initial condition of the electrolyte potential
LICS	Initial concentration of lithium in the solid particles
CURRIC	Initial current of the cycle operation
FLUXIC	Initial pore wall flux
PHI2	Initial condition of the electrode potential

BATTERY**BATTERY_ECHEM_MAT_ANODE*****BATTERY_ECHEM_MAT_ANODE**

Purpose: Set the battery material variables for the anode side electrode.

Card 1	1	2	3	4	5	6	7	8
Variable	PIDA	IOCPA	CAPTA	SOCA	RADA	RATEA	RANODE	
Type	I	I	F	F	F	F	F	
Default	none	none	none	none	none	none	none	

Card 2	1	2	3	4	5	6	7	8
Variable	RHOEA	RHOFA	RHOCCA	DFSA	COND A	MWA		
Type	F	F	F	F	F	F		
Default	none	none	none	none	none	none		

Card 3	1	2	3	4	5	6	7	8
Variable	VFEA	VFPA	VFFA	VFGA				
Type	F	F	F	F				
Default	none	none	none	none				

VARIABLE**DESCRIPTION**

PIDA

Part ID

IOCPA

Material type for the OCP in the anode electrode:

EQ.1: Sony carbon (petroleum coke)

EQ.2: MCMB 2510

EQ.3: MCMB 2528

VARIABLE	DESCRIPTION
	EQ.4: KS6 graphite
CAPTA	Coulombic capacity of anode material (units: mAh/g)
SOCA	Initial lithium stoichiometric coefficient of the anode side active material. For example, Li_xC_6 ($0 < x < 0.7$).
RADA	Radius of spherical particles in the anode side active material (units: m)
RATEA	Reaction rate constant for the anode electrode
RANODE	Film resistance for the anode electrode
RHOEA	Density of anode insertion material (electrode particles) (kg/m ³)
RHOFA	Density of the inert filler in the anode (units: kg/m ³)
RHOCCA	Density of the current collector in the anode (units: kg/m ³)
DFSA	Diffusion coefficient of lithium ions in the anode electrode material (units: m ² /s)
COND A	Effective electronic conductivity of the anode porous electrode (units: S/m)
MWA	Molecular weight of the anode electrode (units: kg/mol)
VFEA	Volume fraction of electrolyte in the anode electrode
VFPA	Volume fraction of the polymer phase in the anode electrode
VFFA	Volume fraction of the inert filler in the anode electrode
VFGA	Volume fraction of the gas in the anode electrode

BATTERY**BATTERY_ECHEM_MAT_CATHODE*****BATTERY_ECHEM_MAT_CATHODE**

Purpose: Set the battery material variables for the positive electrode.

Card 1	1	2	3	4	5	6	7	8
Variable	PIDC	IOCPC	CAPTC	SOCC	RADC	RATEC	RCATHDE	
Type	I	I	F	F	F	F	F	
Default	none	none	none	none	none	none	none	

Card 2	1	2	3	4	5	6	7	8
Variable	RHOEC	RHOFC	RHOCCC	DFSC	COND C	MWC		
Type	F	F	F	F	F	F		
Default	none	none	none	none	none	none		

Card 3	1	2	3	4	5	6	7	8
Variable	VFEC	VFPC	VFFC	VFGC				
Type	F	F	F	F				
Default	none	none	none	none				

VARIABLE**DESCRIPTION**

PIDC Part ID

IOCPC Material type for the open-circuit potential:
 EQ.1: Mn₂O₄(lower plateau) (1.1 < y < 1.99)
 EQ.2: Mn₂O₄ (upper plateau) (0.17 < y < 0.99)
 EQ.3: Cobalt dioxide 1, Li_yCoO₂ (0.0 < y < 0.99)

VARIABLE	DESCRIPTION
	EQ.4: Cobalt dioxide 2, Li_yCoO_2 ($0.0 < y < 0.99$)
	EQ.5: Mn_2O_4 (literature version) ($0.17 < y < 0.99$)
	EQ.6: NMC-111
	EQ.7: NMC-811
CAPTC	Coulombic capacity of the cathode material (units: mAh/g)
SOCC	Initial lithium stoichiometric coefficient for the cathode side active material. For example, Li_yWO_3 ($0 < y < 0.67$).
RADC	Radius of spherical particle in the cathode side active material. (units: m)
RATEC	Reaction rate constant for the cathode electrode
RCATH	Film resistance for the cathode electrode
RHOEC	Density of the cathode insertion material (electrode particles). (units: kg/m ³)
RHOFC	Density of the cathode side inert filler (units: kg/m ³)
RHOCCC	Density of the cathode side current collector (units: kg/m ³)
DFSC	Diffusion coefficient of lithium ions in the cathode insertion material (units: m ² /s)
CONDC	Effective electronic conductivity of the cathode porous electrode (units: S/m).
MWC	Molecular weight of the cathode electrode (units: kg/mol)
VFEC	Volume fraction of electrolyte in the cathode electrode
VFPC	Volume fraction of the polymer phase in the cathode electrode
VFFC	Volume fraction of the inert filler in the cathode electrode
VFGC	Volume fraction of the gas in the cathode electrode

*BATTERY

*BATTERY_ECHEM_MAT_ELECTROLYTE

*BATTERY_ECHEM_MAT_ELECTROLYTE

Purpose: Set the battery material variables for the electrolyte and separator.

Card 1	1	2	3	4	5	6	7	8
Variable	PIDEL	IOPCE	IELTYPE	RHOEL	RHOP	RHOS		
Type	I	I	I	F	F	F		
Default	none	none	none	none	none	none		

Card 2	1	2	3	4	5	6	7	8
Variable	VFES	VFPS	VFGS					
Type	F	F	F					
Default	none	none	none					

VARIABLE	DESCRIPTION
PIDEL	Part ID
IOPCE	Material type for the open-circuit potential: EQ.1: LiPF6 in EC : DMC (1:1). EQ.2: LiPF6 in EC : DMC (2:1). EQ.3: LiPF6 in EC : DMC (1:2). EQ.4: LiPF6 in PC EQ.5: LiClO4 in PC Here, EC is ethylene carbonate, DMC is dimethyl carbonate, and PC is propylene carbonate.
IELTYPE	Type of electrolyte (units: kg/m ³): EQ.0: Liquid electrolyte EQ.1: Polymer electrolyte

VARIABLE	DESCRIPTION
RHOEL	Density of the electrolyte (units: kg/m ³)
RHOP	Density of the polymer phase (units: kg/m ³)
RHOS	Density of the separator material (units: kg/m ³)
VFES	Volume fraction of electrolyte in the separator
VFPS	Volume fraction of the polymer phase in the separator
VFGS	Volume fraction of the gas in the separator

BATTERY**BATTERY_ECHEM_THERMAL*****BATTERY_ECHEM_THERMAL**

Purpose: Set parameters for the thermal treatment in a cell stack.

Card 1	1	2	3	4	5	6	7	8
Variable	TNAME	ITTYPE	IPRT	CP	HCONV	TEMP		
Type	A	I	I	F	F	F		
Default	none	none	none	none	none	none		
Remarks			3	2	2	2		

Card 2	1	2	3	4	5	6	7	8
Variable	FILE							
Type	A							

VARIABLE	DESCRIPTION
TNAME	Thermal material identifier
ITTYPE	Flag for how temperature is determined: EQ.0: Constant temperature mode EQ.1: Isothermal temperature with time EQ.2: Thermal coupling with LS-DYNA thermal solver
IPRT	Data print in ASCII format: EQ.0: No data print out. EQ.1: Time versus heat flux print out for thermal solver
CP	Specific heat coefficient of the cell (units: J/(kg K))
HCONV	Convective heat transfer coefficient with external medium. (units: W/(m ² K))
TEMP	Ambient temperature around the cell stack (K)

VARIABLE	DESCRIPTION
FILE	Name of the battery cell output file (ASCII)

Remarks:

- Battery Parts for Thermal-Mechanical Coupling.** In case of thermal-mechanical coupling, the part number for the battery simulation must be specified, so only this part number is considered in the battery parts.
- Material Properties for Thermal-Mechanical Coupling.** If ITTYPE is 2, the material properties are set through the thermal material card, including anisotropic conductivities (see *MAT_THERMAL_ORTHOTROPIC). CP, HCONV, and TEMP specified here are ignored.
- Heat Flux Output.** If IPRT = 1, then the heat flux generated by the battery solver is printed out.

Example:

The following is a partial example for 1D Electrochemistry.

```
*Keyword
$
*TITLE
1D battery models
$
*BATTERY_ECHEM_CONTROL_SOLVER
$-----1-----2-----3-----4-----5-----6-----7
$ imodel    idimen    ncycle    iaging    itra      igas
$      2          1          1          1          1          1
$ cmode      ctype     cend      tcut      vcut      rcurr
$      0          0          2          0.0        3.0        8.75
$ aging cards
$   seimw    seirho    seibrug    seieps    seic0      seit0
$       0.0      0.0      0.0      0.0      0.0      0.0
$   seii0    seirkka    seicon     ecc0      ecdfs
$       0.0      0.0      0.0      0.0      0.0
$ thermal runaway cards
$   afi       eat       hofec     hofli     hofled
$       0.0      0.0      0.0      0.0      0.0
$   hofc2h4   hoflc     hofco2    hofo2
$       0.0      0.0      0.0      0.0
$ gas initial conditions card
$   ic2h4     io2       ico2     ih2o      ag1       ag2       eg1       eg2
$   1.0e-10   1.0e-10   1.0e-10   1.0e-10   0.0       0.0       0.0       0.0
*CHEMISTRY_BATTERY
battery.inp
btherm.dat
btran.dat
$
*BATTERY_ECHEM_INITIAL
$-----1-----2-----3-----4-----5-----6-----7
$   dt0      lice      phil     lics      curric   fluxic     phi2
$   0.02     1000.0    0.0      0.05     0.0       5.0      -1.0e-7
$
```

*BATTERY

*BATTERY_ECHEM_THERMAL

```
*BATTERY_ECHEM_CELL_GEOMETRY
$-----1-----2-----3-----4-----5-----6-----7
$ imodel      alen      slen      clen      acrlen      ccrlen
      2      9.6e-5    2.5e-5    6.0e-5     1.0e-5     1.0e-5
$ nelea       neles      nelec
      40        40        80
$
*BATTEERY_ECHEM_MAT_ANODE
$-----1-----2-----3-----4-----5-----6-----7
$ pida       i0cpa      capta      soca      rada      ratea      ranode
      2          3      372.0      0.6     8.0e-6    3.0e-9    0.35e-2
$ rhoea       rhofa      rhocca      dfsa      conda      mwa
      1800.0    1800.0    8954.0    7.0e-14   100.0      0.079
$ vfec        vfpc       vffc       vfgc
      0.4        0.0       0.064      0.0
$
*BATTEERY_ECHEM_MAT_CATHODE
$-----1-----2-----3-----4-----5-----6-----7
$ pidc       iocpc      captc      socc      radc      ratec      rcathde
      2          3      274.0      0.8     5.0e-6    3.0e-9      0.0
$ rhoec       rhofc      rhoccc      dfsc      condc      mwc
      5010.0    1800.0    2707.0    3.0e-14    0.5      0.9787
$ vfelc       vfplc      vffic      vfgsx
      0.36        0.0       0.106      0.0
$
*BATTEERY_ECHEM_MAT_ELECTROLYTE
$-----1-----2-----3-----4-----5-----6-----7
$ pidel       iocpe      ieltype      rhoel      rhop      rhos
      2          1          0     1324.0    1780.0    552.0
$ vfels       vfpls      vfgss
      0.4        0.0       0.0
$
*BATTERRY_ECHEM_THERMAL
$-----1-----2-----3-----4-----5-----6-----7
$ tname      ittype      iprt      cp      hconv      temp
  hot_batt      1          0      500.0      0.0     298.15
heat_discharg_lco.k
$END
```