

# **\*BATTERY**

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

- \*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**

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.

| <b>VARIABLE</b> | <b>DESCRIPTION</b>   |
|-----------------|--|
|                 | 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 | CCCLLEN |   |   |
| 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 <a href="#">Remark 1</a> ) |
| 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                 |
| CCCLLEN | 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        |

| <b>VARIABLE</b> | <b>DESCRIPTION</b>                                  |
|-----------------|---|
| 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 |  |  |
|-------|--------|---------|--------|-------|-------|--|--|

**Card 3.2.** Include this card if IAGING = 1.

|       |        |        |      |       |  |  |  |
|-------|--------|--------|------|-------|--|--|--|
| SEIIO | SEIRKA | SEICON | ECC0 | ECDFS |  |  |  |
|-------|--------|--------|------|-------|--|--|--|

**Card 4.1.** Include this card if ITRA = 1.

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

**Card 4.2.** Include this card if ITRA = 1.

|        |       |        |       |  |  |  |  |
|--------|-------|--------|-------|--|--|--|--|
| HOF2H4 | HOF2C | HOF2O2 | HOF2O |  |  |  |  |
|--------|-------|--------|-------|--|--|--|--|

**Card 5.** Include this card if IGAS = 1.

|       |     |      |      |     |     |     |     |
|-------|-----|------|------|-----|-----|-----|-----|
| IC2H4 | IO2 | ICO2 | IH2O | AG1 | AG2 | EG1 | EG2 |
|-------|-----|------|------|-----|-----|-----|-----|

#### 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   | <p>Sets the battery model:</p> <p>EQ.1: Dual insertion model (Newman). IAGING, ITRA, and IGAS must be set to 0.</p> <p>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 <a href="#">Remark 1</a>.</p> <p>EQ.3: Lithium metal battery</p> |
| IDIMEN   | <p>Sets the geometric dimension:</p> <p>EQ.1: 1D LIB models</p> <p>EQ.101: 1D models with thermo-mechanical coupling (available for IMODEL = 1 and 2). See <a href="#">Remark 2</a>.</p>  |
| NCYCLE   | Number of cycles to run. Default is 1 cycle.  |
| IAGING   | <p>Aging model flag (see <a href="#">Remark 3</a>):</p> <p>EQ.0: Off</p> <p>EQ.1: On</p>  |
| ITRA     | <p>Thermal runaway model flag (see <a href="#">Remark 3</a>):</p> <p>EQ.0: Off</p> <p>EQ.1: On</p>  |
| IGAS     | <p>Gas generation model flag (see <a href="#">Remark 4</a>):</p> <p>EQ.0: Off</p> <p>EQ.1: On</p>   |

## \*BATTERY

## \*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 | SEIC0 | SEIT0 |   |   |
| 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  |
| SEIC0   | Initial SEI concentration (units: mol/m <sup>3</sup> )                                  |
| SEIT0   | 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. |

| <b>VARIABLE</b> | <b>DESCRIPTION</b>          |
|-----------------|-----------------------------|
| ECDFS           | 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 | HOFECE | 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   |   |   |   |   |

| <b>VARIABLE</b> | <b>DESCRIPTION</b>   |
|-----------------|--|
| AFI             | Frequency factor for the reaction  |
| EAT             | Activation energy for the reaction   |
| HOFECE          | 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 <sub>2</sub> CO <sub>3</sub> ; units: kJ/mol) |
| HOFCO2          | Formation enthalpy of CO <sub>2</sub> (units: kJ/mol)                      |
| HOFO2           | Formation enthalpy of O <sub>2</sub> (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 <sub>2</sub> H <sub>2</sub> gas (units: mol/m <sup>3</sup> ) |
| IO2   | Initial concentration of O <sub>2</sub> gas (units: mol/m <sup>3</sup> )                |
| ICO2  | Initial concentration of CO <sub>2</sub> gas (units: mol/m <sup>3</sup> )               |
| IH2O  | Initial concentration of H <sub>2</sub> O gas (units: mol/m <sup>3</sup> )              |
| 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:**

1. **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.
2. **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.
3. **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**

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 | CONDA | 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



| <b>VARIABLE</b> | <b>DESCRIPTION</b>  |
|-----------------|---|
|                 | 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, $\text{Li}_x\text{C}_6$ ( $0 < x < 0.7$ ). |
| 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) ( $\text{kg}/\text{m}^3$ )  |
| RHOFA           | Density of the inert filler in the anode (units: $\text{kg}/\text{m}^3$ )   |
| RHOCCA          | Density of the current collector in the anode (units: $\text{kg}/\text{m}^3$ )  |
| DFSA            | Diffusion coefficient of lithium ions in the anode electrode material (units: $\text{m}^2/\text{s}$ )                                 |
| CONDA           | Effective electronic conductivity of the anode porous electrode (units: $\text{S}/\text{m}$ )   |
| MWA             | Molecular weight of the anode electrode (units: $\text{kg}/\text{mol}$ )  |
| 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 | IOPC | CAPTC | SOC  | 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 | CONDC | 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

IOPC

Material type for the open-circuit potential:

EQ.1:  $\text{Mn}_2\text{O}_4$ (lower plateau) ( $1.1 < y < 1.99$ )

EQ.2:  $\text{Mn}_2\text{O}_4$  (upper plateau) ( $0.17 < y < 0.99$ )

EQ.3: Cobalt dioxide 1,  $\text{Li}_y\text{CoO}_2$  ( $0.0 < y < 0.99$ )

| VARIABLE | DESCRIPTION  |
|----------|--|
|          | EQ.4: Cobalt dioxide 2, $\text{Li}_y\text{CoO}_2$ ( $0.0 < y < 0.99$ )   |
|          | EQ.5: $\text{Mn}_2\text{O}_4$ (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, $\text{Li}_y\text{WO}_3$ ( $0 < y < 0.67$ ). |
| 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 <sup>3</sup> )   |
| RHOFC    | Density of the cathode side inert filler (units: kg/m <sup>3</sup> )   |
| RHOCCC   | Density of the cathode side current collector (units: kg/m <sup>3</sup> )  |
| DFSC     | Diffusion coefficient of lithium ions in the cathode insertion material (units: m <sup>2</sup> /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 | IOCPE | 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

IOCPE

Material type for the open-circuit potential:

EQ.1: LiPF<sub>6</sub> in EC : DMC (1:1).

EQ.2: LiPF<sub>6</sub> in EC : DMC (2:1).

EQ.3: LiPF<sub>6</sub> in EC : DMC (1:2).

EQ.4: LiPF<sub>6</sub> in PC

EQ.5: LiClO<sub>4</sub> in PC

Here, EC is ethylene carbonate, DMC is dimethyl carbonate, and PC is propylene carbonate.

IELTYPE

Type of electrolyte (units: kg/m<sup>3</sup>):

EQ.0: Liquid electrolyte

EQ.1: Polymer electrolyte

| <b>VARIABLE</b> | <b>DESCRIPTION</b>  |
|-----------------|---|
| RHOEL           | Density of the electrolyte (units: kg/m <sup>3</sup> )        |
| RHOP            | Density of the polymer phase (units: kg/m <sup>3</sup> )      |
| RHOS            | Density of the separator material (units: kg/m <sup>3</sup> ) |
| VFES            | Volume fraction of electrolyte in the separator               |
| VFPS            | Volume fraction of the polymer phase in the separator         |
| VFCS            | 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:<br>EQ.0: Constant temperature mode<br>EQ.1: Isothermal temperature with time<br>EQ.2: Thermal coupling with LS-DYNA thermal solver |
| IPRT   | Data print in ASCII format:<br>EQ.0: No data print out.<br>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 <sup>2</sup> K))   |
| TEMP   | Ambient temperature around the cell stack (K)  |

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

**Remarks:**

1. **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.
2. **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.
3. **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     seirka     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
$ 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      phi1     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      acclen    ccclen
$         2      9.6e-5    2.5e-5    6.0e-5    1.0e-5    1.0e-5
$   nelea      neles      nelec
$         40      40      80
$
*BATTERY_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      rhoeca      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
$
*BATTERY_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
$
*BATTERY_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
$
*BATTERY_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
```