

Steady/MARC Model Development



Steady/MARC loads by default a "Dense" model, we want to start modifying this "Dense" model into our basic case model



Steady/MARC Model Development



This panel is simply to give the model/project a name and a description for future reference



DOS/MARC Model Development



DOS/MARC is the DOS batch mode equivalent of Steady/MARC; the user defines the model parameters in a file called top.marc instead of using a graphic user interface.

Yet, some features of Steady/MARC have no equivalent in DOS/MARC; the project description may enter in one of them.



Steady/MARC Model Development



The following group of 3 panels are used to enter parameters related to the evaluation of the cell internal heat



Steady/MARC Model Development



$$\rho_{bath} C_p \frac{dT_{bath}}{dt} = \rho_{bath} \frac{dV_{bath}}{dt} + \rho_{bath} \frac{dV_{core}}{dt}$$

$$\rho_{bath} C_p \frac{dT_{bath}}{dt} = \rho_{bath} \frac{dV_{bath}}{dt} + \rho_{bath} \frac{dV_{core}}{dt}$$

Equation that compares the bath or core density

Because the "Dense" model is very similar to our basic case model, there are no need to modify the "Bath Current Density" panel



DOS/MARC Model Development



In DOS/MARC, the model dimensions are defined here:



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Equations that compute the bath resistivity

In the "Bath & Electrolyte Voltage" panel, it is recommended to keep the default
Wright bath resistivity equation to compute the bath resistivity.

DOS/MARC Model Development

In DOS/MARC, the bath resistivity model is selected here.

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Equations that compute the bath voltage

In the "Bath & Electrolyte Voltage" panel, it is recommended to select the
Huang bath voltage equation and use 1.5 for the bath life thickness

DOS/MARC Model Development

In DOS/MARC, the bath voltage model is selected here.

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Equations that compute the electrolyte voltage

In the "Bath & Electrolyte Voltage" panel, it is recommended to select the modified
Huang electrolyte voltage

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In DOS/MARC, the electrolyte voltage model is selected here.

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Equation that compute the current efficiency (Soll)

In the "Obtain Voltages & CE" panel, it is recommended to keep the Solve+ CE model with -1 for the starting slope and 3 as constant.

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In DOS/MARC, only the Solve+ current efficiency mode is available and the 2 extra parameters are defined here:

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Advanced coupling equation

In the "Obtain Voltages & CE" panel, it is recommended to deactivate the advanced coupling option.

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Advanced coupling mode is not available in DOS/MARC

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Equation that compute the cathode drop

In case of using the cathode drop value in the "Obtain Voltages & CE" panel, it is recommended to activate the new cathode drop sub model.

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Equation that compute the cathode drop

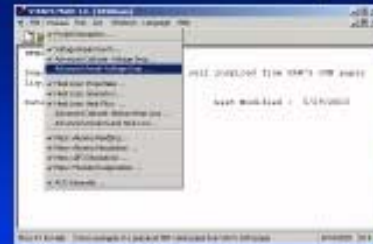
In the "Advanced Cathode Drop" panel, again because the "Dero" model is very similar to our base case model, only the cathode reactivity and the calibration coefficient need to be adjusted.

DOS/MARC Model Development

Cathode drop sub-model is not available in DOS/MARC



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Instead of using the anode drop value in the "Ohmic Voltage & CE" panel, it is recommended to activate the new anode drop sub-model.



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Equations that compute the anode drop

In the "Advanced Anode Drop" panel, again because the "Dense" model is very similar to our base case model, only the reference voltage from front top of anode to anode base need to be adjusted.



DOS/MARC Model Development

Anode drop sub-model is not available in DOS/MARC



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Once the anode and the anode voltage drop sub-models have been activated, the computed values are displayed in the "Ohmic Voltage & CE" panel.



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Line	Value	Unit	Description
1.100	0.000000	1.000000	APPLIED TOP OF ANODE DROPPER IS ALWAYS
1.101	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.102	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.103	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.104	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.105	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.106	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.107	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.108	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.109	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.110	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.111	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.112	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.113	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.114	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.115	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.116	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.117	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.118	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.119	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS
1.120	0.000000	1.000000	TOP OF ANODE DROPPER IS ALWAYS

In DOS/MARC, the anode and anode drop are defined here:



Steady/MARC Model Development



In the "Aluminum/Al oxide" panel, there are nothing to be changed



DOS/MARC Model Development



In DOS/MARC, the equivalent properties are found here



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In the "Elastic" panel, all properties can be adjusted



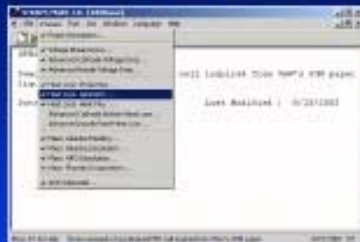
DOS/MARC Model Development



In DOS/MARC, the equivalent properties are found here



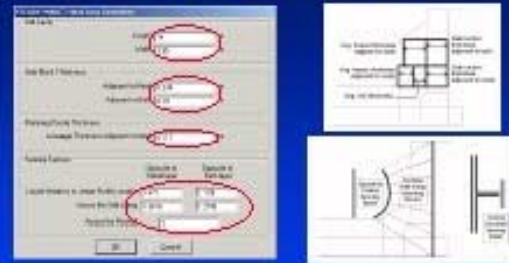
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After the properties adjustment, the next step is adjusting the geometric parameters



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In the "Geometric" panel, all parameters must be adjusted



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Equation that compares the cathode bottom heat loss

In the "Advanced Cathode Heat Loss" panel, again because the "Demand" model is very similar to our base case model, only shell wall heat loss at pier level need to be adjusted

DOS/MARC Model Development

Cathode heat loss sub-model is not available in DOS/MARC

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Instead of fixing the anode panel heat loss value in the "Heat Flux" panel, it is recommended to activate the new anode panel heat loss sub-model

Steady/MARC Model Development

Equations that compare the anode panel heat loss

In the "Advanced Anode Panel Heat Loss" panel, again because the "Demand" model is very similar to our base case model, only a few parameters need to be adjusted

DOS/MARC Model Development

Anode panel heat loss sub-model is not available in DOS/MARC

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Once the cathode bottom and the anode panel heat loss sub-models have been activated, the compared values are displayed in the "Heat Flux" panel

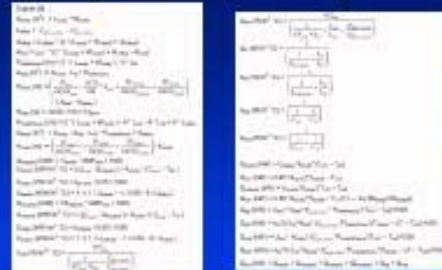
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Code	Symbol	Unit	Description
1.0002	Q2C	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF BASE LEVEL
1.0003	Q2D	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0004	Q2E	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0005	Q2F	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0006	Q2G	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0007	Q2H	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0008	Q2I	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0009	Q2J	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0010	Q2K	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0011	Q2L	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0012	Q2M	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0013	Q2N	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0014	Q2O	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0015	Q2P	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0016	Q2Q	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0017	Q2R	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0018	Q2S	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0019	Q2T	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0020	Q2U	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0021	Q2V	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0022	Q2W	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0023	Q2X	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0024	Q2Y	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE
1.0025	Q2Z	EW/WT	THEORETICAL EFFICIENCY OF THE DRAIN OF THE DRAINAGE

In DOS/MARC, the cathode and anode drop are defined here:



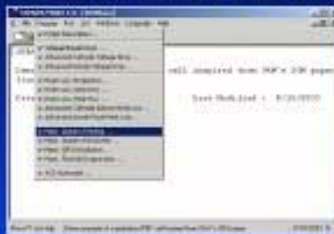
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At this stage, we are done defining the parameters specifically related to the calculation of the cell heat loss.



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The following group of 4 panels are used to enter parameters related to the evaluation of the cell different anode balances. We can skip them for now as the advanced sampling options are not active (no impact on heat balance).



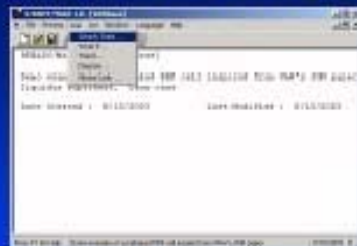
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The last panel in the Process drop-down menu is used to enter parameters related to the evaluation of the ACD menu. We can also skip it for now as the advanced sampling options are not active (no impact on heat balance).



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The final panel in the Run drop-down menu.



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Any parameters in that panel can be selected to be the "Target" variable to converge the steady state conditions. Often, it is very convenient to select the concentration of dissolved aluminum in the bath as a target variable.



