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Sequential Simulation in COMSOL Using Differential Equations to Perform Digital Switching

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Abstract: COMSOL facilitates the simulation of complex, cross-linked partial differential equations with static boundary conditions in the time-domain. However, the lack of a sequential simulation solver that can dynamically adopt new boundary conditions irreversibly based on calculated physical parameters can make certain simulations challenging. In this paper, a differential equation based method to create a 2-state switching mechanism for the boundary condition is presented, using the charge cycle of a lithium ion battery simulation as an example. The result is a one-way, smooth transition between different operation states. This method can also be extended to more complex models with more states and also for cyclic processes.

Keywords: sequential simulation, switching,

1. Introduction:

Many physical systems contain sequential modes of operation. The sequence is one-way and switching between modes is dependent upon specific internal parameters of the system itself. While COMSOL provides the flexibility to perform time-domain simulation and time-based modifications of boundary conditions, simulating sequential systems based on internal physical variables in COMSOL can be a formidable challenge due to the lack of a built-in method to sequentially change boundary conditions based on calculated parameters. For example, a lithium ion battery's charge and discharge cycle has three distinct, sequential states: discharge, constant current charge and constant voltage charge. The switching between these three states is determined by the cell voltage reaching specific upper and lower boundaries as shown in Figure 1. Depending on the discharging and charging conditions, the time at which these switching conditions are reached is variable, and simple conditional statement based boundary conditions would cause switching back and forth between the states due to instantaneous feedback state chatter. All of these system characteristics and the manner COMSOL is normally configured directly prevent the simulation of such systems in a straightforward fashion.

In this paper, a systematic, differential equation based approach that allows the simulation of such sequential state machines is presented. The methodology also allows both distinct, digital type switching between states and switching while allowing a specific simulated parameter to settle asymptotically to a specific value. A simplified example, two of the three states, in the aforementioned battery cycling problem is used to illustrate the methodology.

2. Methodology:

The description of the methodology assumes a time-dependent problem with a single boundary condition to be controlled based on one calculated physical parameter. However, it can be easily extended to models with multiple changing boundary conditions and multiple calculated internal physical parameters.

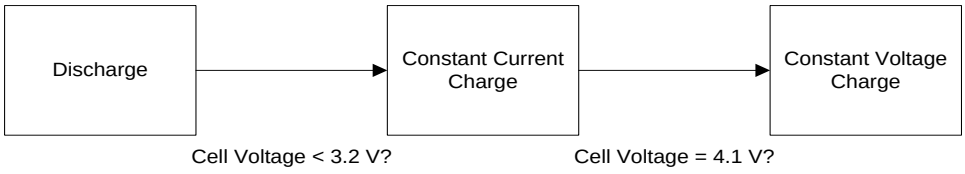

Figure 1. The lithium ion battery discharge/charge cycle, as a three-state, two-switch state machine.

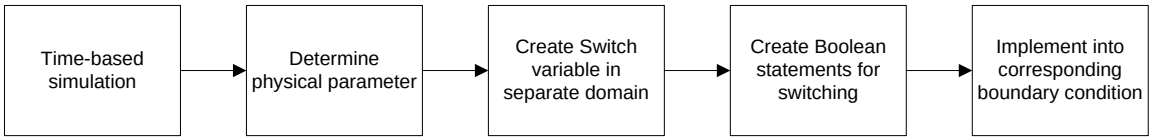

Figure 2. The four-step differential equation based switching process

Making use of the fact that COMSOL is an efficient solver for differential equations, the key concept is to define the behavior of the switching variable through a first-order differential equation and use the impulse response generated by the computed internal physical parameter hitting a pre-defined limit and integrating it to produce a step-function. This step function is then used in as a conditional statement in the boundary condition that needs to be switched.

A typical time-based discharge/charge curve for a lithium battery is shown in Figure 3.

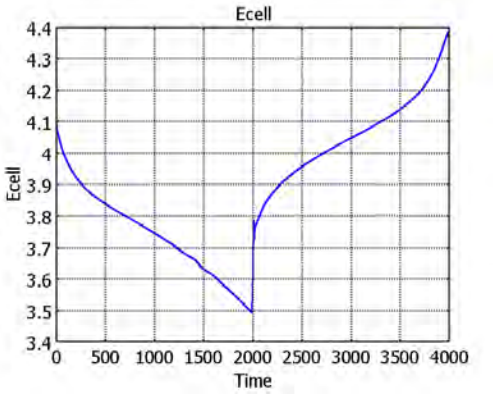

Figure 3, The lithium ion battery discharge/charge cycle, as a three-state two-switch state machine

In this simulation, the boundary condition, current applied, was changed arbitrarily at t = 2000 sec. However, this limits the model from simulating higher current discharge, which would cause the cell voltage (ECell) to plummet below physical limits. In another words, the end-of-discharge voltage limit was arbitrary, which could also present a consistency issue if this model is cycled. A time-based simulation would form a good starting point of the conditionally switched model. The base model we used for this modification is included in the COMSOL 3.5 Chemical Engineering Module's Model Library named "li battery"[1]. This model was based on the work of Newman[2]. While this model was developed under version 3.5, it is equally applicable to version 4 of COMSOL using the new interface.

The approach is a four-step process as shown in Figure 2

Step 1. First, the physical parameters that govern all the switching are defined. In the example, it is desired that the lithium ion battery switches from discharge mode to charge mode when the cell potential reaches a 3.2 V lower limit.

Upon hitting the preset cell voltage limit, the boundary condition, applied current in this case, is to be changed. The simplified charge/discharge cycle is shown in Figure 4. This is a two-state state machine, and requires only a 1-bit switch. A four-state machine would require 2-bits, and so on.

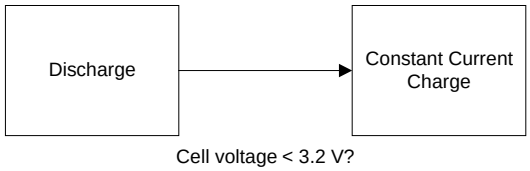

Figure 4. The simplified, two-state 1-bit switch, state machine

Step 2. Having defined the physical parameter, the second step is to assign an arbitrary variable to be integrated. This variable is then implemented in a unit length subdomain, separate from the actual physical model. The subdomain's expression is then set to:

$$\frac{dSwitch}{dt} = flc1hs(3.2 - Ecell, 0.1) \times flc1hs(50 - Switch, 0.1) \times rate$$

where Ecell is the cell voltage, a coupling variable calculated from the physics of the battery. The first part of the equation provides a smoothed Heaviside step when the switching condition is met at 3.2 V. The Heaviside function is used to improve convergence over a simple conditional statement. The second part of the equation sets up an arbitrary upper limit that the value Switch will attain. The variable *rate*

provides a multiplier to control the speed of switching. Both the limit and the rate are arbitrary values that can be adjusted for specific physics. This expression is plotted against time in Figure 5.

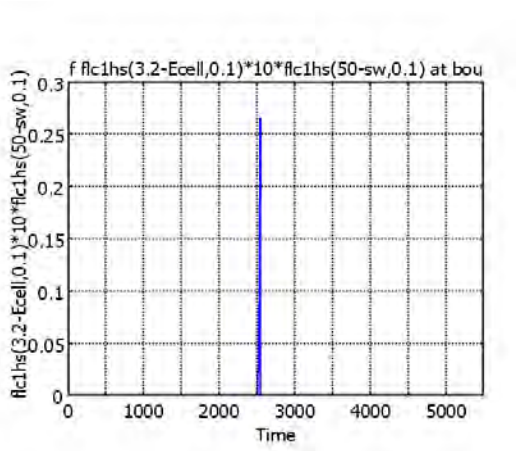

Figure 5. Pulse generated by the subdomain expression for Switch.

For this arbitrary Switch variable, all of the boundary conditions in the subdomain are set to 0 (insulation), with initial value 0.

As the calculated physical value (Ecell) reaches the limit of 3.2 V, the Heaviside function generates a positive pulse, which is integrated into a step function that is bounded to the high limit (50 in this case), shown in Figure 6. Since there is no other function to produce a negative pulse, the value of Switch remains high over time. An integral coupling variable "IntSwitch" (integral of Switch over the unit length domain) can then be used to carry the step function back to the physical domain for calculations.

Step 3. Using IntSwitch, two distinct Boolean variables can be created in scalar expressions.

Discharge=flc1hs(25-IntSwitch,0.05)
Charge=flc1hs(IntSwitch-25,0.1)

The *Discharge* state is true when the value IntSwitch is less than 25, while Charge is true when it is over 25. 25 is chosen as the mid-point between 0 and 50. The range in the Heaviside functions differs intentionally to provide asymmetrical switching time for the two Boolean variables. This is needed to prevent chatter between states, and improve convergence. This value is only an initial choice for testing purposes in the time-based simulation. It would likely require adjustments after the implementation of the switch into the boundary condition.

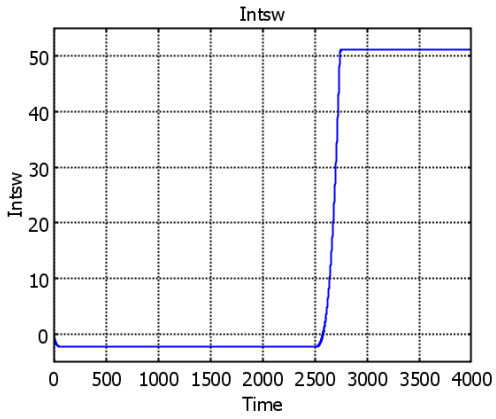

Figure 6. Pulse integrated to become a non-reversible step function with adjusted conditions.

Step 4. The two variables can then be implemented into the boundary condition. In this application, the boundary condition is an applied current i_app.

$$i_{app} = i_{discharge} \times Discharge + i_{charge} \times Charge$$

where *i_discharge* and *i_charge* are current constants in Amps (A).

It should be noted that upon adding the conditional statement to the boundary condition, there is now a dynamic feedback in the system and the boundary condition is now independent of time. This invariably will change the value and the width of the pulse generated by the Heaviside function in Step 2, which would subsequently produce a value for Switch that may or may not be bounded by the limit (50 in the example) and the *rate* variable should be adjusted to create a usable step function. In this example, the initial *rate* created a step function between 0 and just over 1, as shown in Figure 7.

To make this usable for the conditional statements, the mid-point was adjusted from 25 to 0.5 for the two Boolean variables.

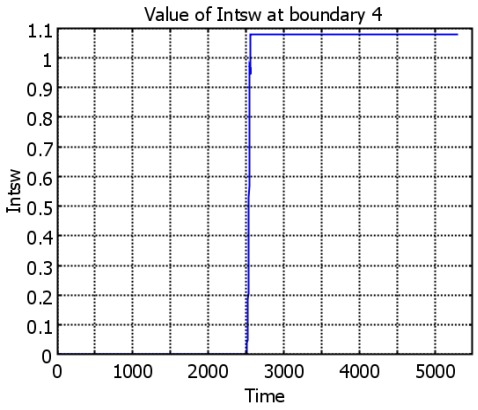

Figure 7. New IntSwitch value after implementing conditional applied current into boundary condition.

Discharge=flc1hs(0.5-IntSwitch,0.05)
Charge=flc1hs(IntSwitch-0.5,0.1)

With this adjustment, the setup for the dynamic switching simulation is complete.

In this example,

i_discharge = -i_charge = 17.5,

and the applied current boundary condition is shown in Figure 8.

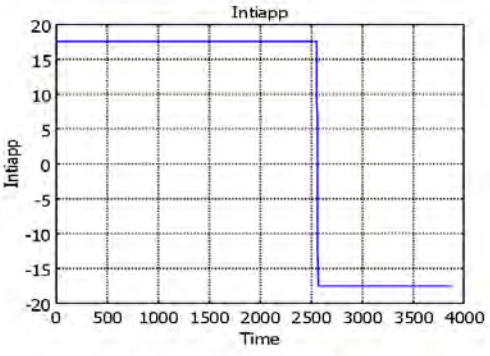

Figure 8. Discharge and charge current based on conditional switching.

Using this boundary condition, the charge and discharge curve was simulated, and the result is shown in Figure 9.

At time = 2651 s, the current switched within a period of about 10 s. The voltage step corresponded to the Ohmic drop, and the subsequent increase is due to constant current charging. The behavior is identical to the time-based simulation. There is a small amount of settling time within the switching period, but convergence was obtained.

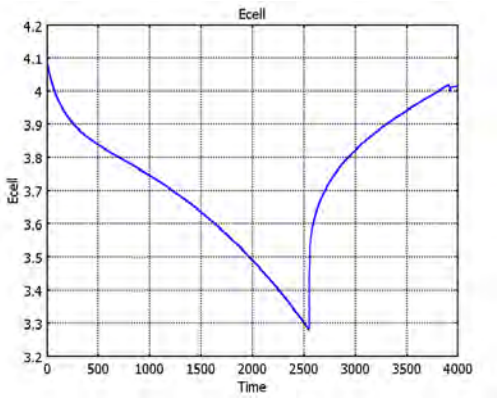

Figure 9. Discharge-charge voltage curve based on conditional switching.

3. Discussion

While the four-step process described above involved a single switching event, it can be extended to systems involving multiple conditions simply by adding more arbitrary "switch physics" into the unity length subdomain and creating the table of boundary conditions to the corresponding "logic states". The three steps after the definition provide much needed flexibility such that each of the switching events can be tailored to fit each specific physical condition. The size of the impulse function can be adjusted by changing the *rate* and the Heaviside function's *range* variable in the subdomain expression in step 1. The switches can also be customized to fit the output of the integrated step function before it is implemented into the boundary expression of the physical variable of the model.

It should be noted that the adjustment of the *rate* and the conditional statement Boolean variables to obtain proper switching is an iterative process which must be adaptively refined once the conditions are implemented into the physical subdomain as a boundary condition. This dynamic feedback also requires that the sequence of the events be considered. The asymmetry of the switching statements is needed to generate hysteresis, thus producing a one-way and irreversible change that is free from non-convergent simulation chatter.

4. Summary

A method of sequential simulation through digital switching using differential equations has been presented. The method creates an isolated, artificial subdomain with an arbitrary variable that is used as a switch, whose value is derived from pre-determined physical limits placed upon computed internal physical variables.

5. Acknowledgments

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6. References

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[1] R. Darling and J. Newman, "Modeling Side Reactions in Composite $Li_yMn_2O_4$ Electrodes", *J. Electrochem. Soc.*, **vol. 145**, pp. 990 (1998).