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CASL-U-2015-0166-000

CRUD Modeling in MPACT

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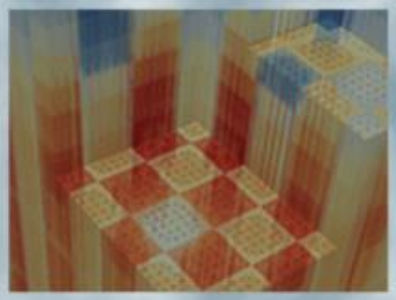

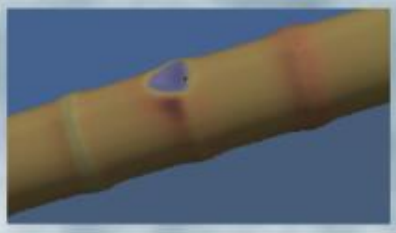

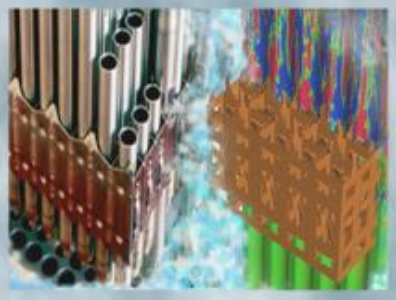

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REVISION LOG

Revision	Date	Affected Sections	Revision Description
Rev. 0	5/22/2015	All	Initial release

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ACRONYMS

CASL	Consortium for Advanced Simulation of Light Water Reactors
CIPS	CRUD Induced Power Shift
CTF	COBRA-TF
HPC	high-performance computing
LWR	light water reactor
ORNL	Oak Ridge National Laboratory
PCM	percent mille (10^{-5})
PWR	pressurized water reactor
RTM	Radiation Transport Methods
T-H	thermal-hydraulics
TPL	third-party library
VERA	Virtual Environment for Reactor Applications

1 Introduction

One of the challenge problems in CASL is to better understand the effects of CRUD on PWRs. One of the primary focuses of the CRUD work this year is the ability to simulate CRUD Induced Power Shift (CIPS). In order to meet this requirement, VERA-CS is being modified in order to model the space and time dependent deposition of CRUD onto the fuel and capture the effects it has on the local power and thermal hydraulic conditions in the core.

Several contributions to the CRUD work have been achieved over the past several in CASL. One of the first was the tight coupling of ANC, VIPRE, and BOA [#]. This was followed by several developments of the MAMBA code [#] and the coupling of MAMBA to DeCART and Star-CCM+ [#]. More recently, MAMBA has been coupled with Hydra-TH [#].

This work is a small piece of the CIPS mission for CASL this year. The coupling of the subchannel thermal hydraulics code CTF to the coolant chemistry code MAMBA has been demonstrated [#]. This work allows CTF to call MAMBA and grow CRUD on the surface of every fuel pin in the core given a fixed power history. The two upcoming milestones (L2:PHI.P11.01 and L1:CASL.P11.03) focus on using VERA-CS to simulate multiple cycles of operation and then qualifying the capability for the CIPS challenge problem.

Here, the focus will be on preliminary modeling of the CRUD layer on the surface of the pins and the effect on the neutron transport solution obtained by MPACT. The methodology is added to MPACT to model the CRUD mass deposited on the surface of each pin and the effect on the local power distribution because of the boron present in the $Li_2B_4O_7$ deposits in the CRUD and water displacement caused by the $NiFe_2O_4$ deposits. The process to model the CRUD is then used to understand the sensitivity to meshing parameters for light, moderate, and heavy CRUD deposits. Finally, the plan for the coupling of the three physics is outlined.

2 Uniform CRUD Layer Modeling

The first step to modeling CRUD using MPACT is to generate the infrastructure to smear to the CRUD into a ring on the outside of the fuel element. In order to prevent the need to modify the mesh in MPACT as the CRUD grows, a fixed set of concentric rings is input on the surface of the fuel. The CRUD is then homogenized onto the mesh using volume homogenization.

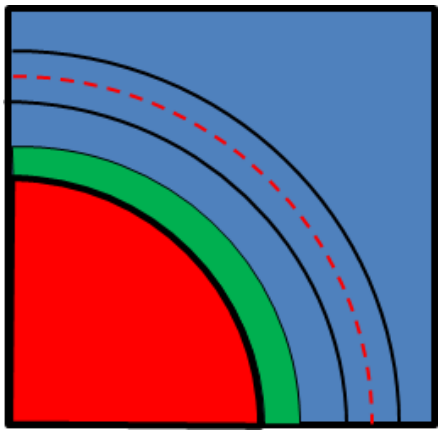

Figure 1: CRUD Regions on a Pin Cell

The CRUD region is to be homogenized into the rings in MPACT. In the figure above, the black lines represent the radial mesh on a pin cell (r_i) and the red dotted line represents the growth of the CRUD region ($r_{clad} + t_{CRUD}$). The first region outside the cladding is completely filled with CRUD and the density of nickel ferrite and boron can be directly applied. The second region partially filled with CRUD, but the remainder is coolant. These two regions must be smeared together. Each region is appropriately volume weighted such that the mass of both the CRUD region and the fluid region are preserved in the volume.

$$\alpha_{CRUD} = \frac{\pi\left(\left(r_{clad}+t\right)^2 - r_i^2\right)}{\pi\left(r_{i+1}^2 - r_i^2\right)} = \frac{\left(r_{clad}+t\right)^2 - r_i^2}{r_{i+1}^2 - r_i^2}$$

In addition to the CRUD being homogenized, it is also porous. This means that the fluid will occupy the porous voids inside the CRUD region. In order to estimate the porosity of the CRUD, the theoretical density of $NiFe_2O_4$ is set to 5.35 g/cm^3 and the density for $Li_2B_4O_7$ is set to 2.44 g/cm^3.

$$P = \frac{\rho_{NiFe_2O_4}}{\rho^{Theoretical}_{NiFe_2O_4}} + \frac{\rho_{Li_2B_4O_7}}{\rho^{Theoretical}_{Li_2B_4O_7}}$$

$$N_{mix} = N_{CRUD} + \left(1 - \alpha_{CRUD} P\right) N_{fluid}$$

The number density of the fluid is straightforward to calculate if the density of the water is known but currently MAMBA does not solve for the volumes of saturated water and vapor in the CRUD layer. The approximation will be made that the bulk coolant temperature is present in the CRUD region unless a better estimate is available. The number density of the CRUD can be calculated directly from the mass of $NiFe_2O_4$ and $Li_2B_4O_7$ which is provided by the coolant chemistry code.

The CRUD model is implemented as a Feedback Operation in the MPACT solver hierarchy. Knowing that eventually a pin-by-pin CRUD region would be needed, the CRUD classes were developed into a base class which can handle the computation of the CRUD layer number density and porosity based on a given $NiFe_2O_4$ and $Li_2B_4O_7$ surface density and thickness. The base class also iterates over the entire mesh, finds the surface of the fuel pins, and homogenizes the CRUD onto the surface of the fuel elements. The extended CRUD classes are only charged with returning the surface density and thickness given a position in the core. For the Uniform CRUD case, this simply means returning the user specified value for every pin. Extensions of this capability can be made to read a distribution from the CTF-MAMBA output file. The final extension will be to directly obtain these values from CTF-MAMBA during the simulation.

3 CRUD Layer Sensitivity Study

In order to understand the meshing requirements needed to simulate CRUD, four different CRUD surface densities were simulated on a single pin cell and a 2D lattice. Theses surface densities represent light, mild, heavy, and extreme CRUD buildup on the fuel. The table below shows the thickness and surface density of $NiFe_2O_4$ and $Li_2B_4O_7$.

Table 1: Simulated CRUD properties

	Thin	Medium	Thick	Extreme
Thickness [microns]	20	50	90	75
$NiFe_2O_4$ Surface density [mg/cm^2]	3.6	10	20	33.24
$Li_2B_4O_7$ Surface density [mg/cm^2]	2.00E-03	0.2	0.4	1.76

The sensitivity on the pin cell is based on VERA Progression Problem 1c [#]. Several cases were run to assess the implementation in addition to the sensitivity of the homogenization of the CRUD layer. The first case uses the developed mechanics to homogenize the CRUD but places a mesh element on the surface of the CRUD so it is explicitly represented. The remaining cases look at increasing the volume in which the CRUD is homogenized and the number of rings used. The CRUD is homogenized into rings of 100, 150, and 200 microns and in addition, the 100 micron case was run with 2 and 4 subdivisions (4 subdivisions of approximately 25 microns to make a total of 100 microns although the rings are divided by equal volume so the spacing is not exactly 25 microns).

In order to understand the sensitivity to the result, the reactivity difference is obtained in pcm for each of the homogenized zones. The reference for this is the first case described above where the CRUD is explicitly meshed.

Table 2: Sensitivity to CRUD for a pin cell
(Differences from non-homogenized CRUD Layer in pcm)

	k-effective	200 (1 subdiv)	150 (1 subdiv)	100 (1 subdiv)	100 (2 subdiv)	100 (4 subdiv)
No CRUD	1.17011	--	--	--	--	--
Thin	1.16872	-4	-5	-4	-4	-4
Medium	1.14484	-9	-7	-4	-2	-2
Thick	1.12067	-16	-7	-1	-1	0
Extreme	0.99792	-108	-40	-15	-7	0

In all cases, the effect on the meshing is minimal. The extreme CRUD case shows the most sensitivity but it is comparable to the error introduced by other meshing choices.

The second case compared is VERA Progression Problem 2c. This is a standard 17x17 PWR assembly with 25 guide tubes. The same regions of uniform CRUD were placed on the surface of the fuel and the eigenvalue is compared in a similar manner as the pin cell. The sensitivity to the pin power is small because of the use of uniform CRUD across the problem.

Table 3: Sensitivity to CRUD for a 2D lattice
(Differences from non-homogenized CRUD Layer in pcm)

	k-effective	200 (1 subdiv)	150 (1 subdiv)	100 (1 subdiv)	100 (2 subdiv)	100 (4 subdiv)
No CRUD	1.173629	--	--	--	--	--
Thin	1.172392	-8	-7	-5	-5	-5
Medium	1.148851	-16	-12	-6	-3	-3
Thick	1.125052	-20	-12	-2	-1	2
Extreme	0.986136	-315	-276	-235	-74	31

Very similar trends can be observed for this case except the extreme CRUD layer incurs considerably higher error. Since the extreme CRUD is not expected to occur on the entire surface of a single fuel pin, and definitely not occur uniformly on an entire assembly, this case should not be considered to be limiting. The suggestion based on these results is that a single 150-200 micron region will provide sufficient accuracy for homogenizing the CRUD layer. This study will need to be repeated with a full distribution of CRUD of varying levels of severity to confirm these results hold for heterogeneous distributions.

4 Plan for Full Core CIPS Calculation

With the initial capability in MPACT to model CRUD on the surface of the pin element and an understanding of the sensitivity of the mesh to different degrees of CRUD deposition, a focus on the path forward to full core CIPS is laid out. Several considerations need to be made; which code will drive the MAMBA subgrid calculation, how will the depletion of the B-10 deposited in the $Li_2B_4O_7$ be modelled, and how will the CRUD data be carried between cycles.

4.1 Three way code coupling

The addition of MAMBA to VERA-CS creates a question on which code best to control the function calls in MAMBA to grow the CRUD layer. Currently MPACT contains the driver code which calls CTF and ORIGEN at the appropriate times during the multistate iteration sequence. MPACT also controls the writing of data to the restart file for the coupled calculation. At first glance, MPACT seems to be the natural place for the MAMBA calls to occur. However previous work has already focused on CTF-MAMBA coupling and CTF already owns the interfaces to call MAMBA. So a strong argument could also be made to leave MAMBA in CTF. In order to determine the best place for MAMBA to be controlled, a study of the data required to be sent to MAMBA and the solution data from MAMBA that are needed by the other physics is performed.

First, an examination of the data needs for MAMBA is performed. Table 4 lists the various data requirements that are needed by MAMBA. In addition, the size of the data and frequency of the need for this data is shown in the respective columns.

Table 4: List of data requirements for MAMBA

MAMBA Needs…	MPACT Has	CTF Has	Size	Type	Frequency
Pressure / Inlet Temp	X	X	2	Scalar	State
Coolant Chemistry	X		5	Scalar	State
Boron	X		1	Scalar	Iteration
Timestep	X		1	Scalar	State
Surface Area	X	X	1	Vector	Initialization
Coolant Temperature		X	1	Vector	Iteration
Heat Flux	X	X	1	Vector	Iteration
Clad Temperature		X	1	Vector	Iteration
Shear Stress		X	1	Vector	Iteration
Restart Info	X		1	Restart	Initialization

Here the state parameters (Pressure, Inlet Temperature, Soluble Li, Soluble Ni, etc) all are known by MPACT because they are input parameters that exist per State. MPACT already passes the pressure and

inlet temperature to CTF at each state because it is needed as boundary conditions for the thermal hydraulics. The boron concentration is a solution variable of MPACT and therefore needs to be passed every iteration. The thermal-hydrualics do not have significant history effect on the time scales that VERA-CS is interested in and therefore MPACT is controlling all of the time step information. MAMBA also needs the surface area for each region in which CRUD is being tracked (currently the desire is to track CRUD on the quarter surface of each pin) but both CTF and MPACT contain the geometric information to calculate this quantity. Finally, several solution variables are needed to be passed during the outer iteration including coolant temperature, heat flux, clad temperature, and shear stress. It should be noted these are needed on the quadrant basis of each pin and therefore, only CTF has this information. The one exception is heat flux, which since CTF is only doing 1D conduction at this time; the power generated is directly proportional to the heat flux on the quadrant surface so MPACT also contains sufficient information to provide this quantity. The last piece of information that MAMBA needs is potentially the restart information from the MPACT restart file. In general, the large data that needs to be passed at every iteration is all owned by CTF.

Secondly, an examination of the data MAMBA needs to provide to CTF and MPACT is shown in Table 5.

Table 5: List of solution data from MAMBA

MAMBA Provides…	MPACT Needs	CTF Needs	Size	Type	Frequency
Thickness	X	Currently	1	Vector	Iteration
Thermal Resistance		X	1	Vector	Iteration
Li2B4O7 Surface Density	X		1	Vector	Iteration
NiFe2O4 Surface Density	X		1	Vector	Iteration
Evaporation Rate		Maybe	1	Vector	Iteration
Restart Info	X		1	Restart	State+

Here, the data is spread evenly between the two codes. CTF only needs the thermal resistance of the crud layer and potentially the evaporation rate. Currently CTF uses the thickness only to convert the resistance to a thermal conductivity, but that is an unnecessary step. MPACT needs the thickness and surface densities for each iteration. MPACT will also need the restart information from MAMBA on request, which could be every state, or less frequently depending on the user input.

Now that the data requirements are understood, it is clear that neither code has enough information to make a clear decision on which code should control MAMBA. A further study is done to determine how much data will need to be passed between the codes depending on which code is driving MAMBA. In order to make this determination, a few assumptions are made about the size of the problem. A quarter core PWR with 49 axial levels in the fuel is assumed which leads to approximately 2.85 million MAMBA cells. In addition, the simulation is assumed to run for 20 states and 12 iterations per state. All of the numbers presented include the passing of scalar data, but has a very minor effect on the total data passed and will be ignored in the discussion. If MPACT is controlling the calls to MAMBA and needs to pass CTF the thermal resistance each iteration and obtain all of the TH properties by quadrant, the total amount of data passed over the course of the simulation would be 20.4 GB. This could be reduced by 1.3 GB because CTF would no longer be required to pass the pin average coolant temperature. If CTF is driving the calls to MAMBA, the total amount of data passed to MPACT from MAMBA is 15.3 GB. This can be reduced to 3.8 GB if CTF only passes the pin average CRUD quantities to MPACT. This makes CTF the clear choice to call MAMBA in order to reduce the total data passed during the simulation. This information along with the fact that the CTF coupling already exists makes this implementation the obvious first step in the implementation.

The restart data that MAMBA provides is a length 580 array of double precision numbers per CRUD region. This data will need to be stored into the restart file that MPACT writes. The total amount of data needed to be passed for the restart file is 12.4 GB. The restart file will likely be written between 5 and 10 times during the simulation along with the initial read of the restart to initialize MAMBA. This means the data passed for the restart will overshadow all other data passed for the coupled solve. At first glance, it might be a sufficient driver for MPACT to control the call to MAMBA in order to reduce the messages passed across the network, but upon careful consideration on how MPACT writes the restart file, it becomes clear that MPACT only writes the restart file on the master process. This means that if the reduction of this data will occur in CTF and MPACT and very little communication will be saved if MPACT controls the calls to MAMBA.

Above, an analysis of the best call sequence for the coupling of MAMBA with VERA-CS was considered. After reviewing the options, it is determined that CTF should call MAMBA. This puts some requirements on the CTF coupling interface to allow for MPACT to pass necessary data to MAMBA and receive data from MAMBA. This data is provided in the list below:

- Ability to specify coolant chemistry values at each state (interface needs to be slightly modified)
- Ability to specify time step at each state (interface needs to be slightly modified)
- Ability to specify boron concentration every coupled iteration
- Ability to return pin average thickness and surface densities

In addition to the above interface requirements, CTF will need to store the MAMBA restart vector at time t_0 and step to time t for every coupled iteration because of the direct impact of power distribution on localized boiling. This is different than the previous work with CTF-MAMBA because in that case, the power was fixed. There are a few extra requirements that are placed on CTF for the restart capability but those will be discussed in section 4.3.

4.2 Depletion

Thus far, the depletion of the CRUD was not considered. Specifically, the boron-10 deposited into the CRUD region will deplete as it is irradiated. This is complicated by the internal physics that are going on in the CRUD layer; the CRUD can erode, more boron from the coolant is being deposited in the CRUD, and some of the precipitated boron will dissolve back into the coolant. All of the physics are not precisely modelled so an approximation needs to be made. The typical correction is to add a multiplier to the removal term in the depletion equation [#]. In addition, the boron-10 concentration in the coolant is depleting. In order to account for both of these effects, a simple model is developed. For the purpose of this demonstration, it is assumed that the boron concentration in the CRUD is increasing.

Consider the crud layer where we know the mass of boron before and after a time step in MAMBA.

$$\delta m_{boron} = m_{boron}\left(t_i\right) - m_{boron}\left(t_{i-1}\right)$$
$$\delta t = t_i - t_{i-1}$$

If change in boron mass is positive.

$$\delta N_B = \frac{\delta m_{boron}}{\alpha_{B10,cool} M_{B10} + \left(1-\alpha_{B10,cool}\right) M_{B11}}$$
$$\delta N_{B10} = \alpha_{B10,cool}\delta N_B$$
$$\delta N_{B11} = \left(1-\alpha_{B10,cool}\right)\delta N_B$$

This takes into account B-10 depletion in the coolant. This does not take into account the depletion of boron in the CRUD layer. We will assume the uptake of boron in the CRUD layer is linear in time, and solve for the depletion of boron in the CRUD layer.

$$\frac{dN_{B10}(t)}{dt} = \left.\frac{dN_{B10}(t)}{dt}\right|_{cool,src} - \gamma\sigma_{a,B10}\phi N_{B10}(t)$$

$$\left.\frac{dN_{B10}(t)}{dt}\right|_{cool,src} = S_{B10} \cong \frac{\delta N_{B10}}{\delta t}$$

$$\frac{dN_{B10}(t)}{dt} = S_{B10} - \gamma\sigma_{a,B10}\phi N_{B10}(t)$$

$$N_{B10}(t) = N_{B10}(0)e^{-\gamma\sigma_{a,B10}\phi t} + \frac{S_{B10}}{\gamma\sigma_{a,B10}\phi}\left(1 - e^{-\gamma\sigma_{a,B10}\phi t}\right)$$

Here γ is the user specified constant which alters the depletion rate of B-10 in the CRUD. The first term here represents the depletion of the B-10 in the CRUD and the second term represents the addition of new CRUD from the coolant and the depletion of that during the time step. A simple extension of this method could be made if the change in mass is negative.

4.3 Restart and Multicycle

The restart and multicycle capability is achieved through routines in MPACT which read and write an HDF5 file throughout the simulation. The multicycle capability also includes the ability to shuffle the fuel between cycles. The presence of CRUD on the surface of the fuel creates a necessary need to store the information needed for MAMBA into the restart file. In section 4.1, the size of the information that MAMBA needs to perform a restart was estimated to be 12.4 GB. Routines are needed in CTF to extract the data for every assembly, every pin, and every quadrant. The hierarchical nature of the restart file allows for data to easily be added. For the CRUD data, it is suggested that a new CRUD block be added to supplement the Assembly and Insert blocks. Then each assembly would be represented into its own folder in the CRUD block. Finally, information about the pin and quadrant would be stored in an efficient manner.

The MAMBA restart data consists of an array of doubles of length 580 and two integers per element. This data needs to be stored on the file in a manner that makes it easy to extract the data during a restart or to shuffle the data before passing the data back to MAMBA. Unlike all of the other shuffling cases experienced thus far, the CRUD has azimuthal dependence. When shuffling the CRUD data, special care needs to be made to correctly rotate or translate the CRUD layers azimuthally as deemed by the boundary conditions. In addition, it might be necessary to have a function in MAMBA that accounts for the shutdown, movement of the fuel, and potential cleaning during the outage. Another option is to assume that all fuel starts out clean at the beginning of the next cycle.

Modifications to MPACT's restart capability are necessary to store the MAMBA restart data files, but special care must be made when saving this data to ensure that memory is not exceeded. For this reason, it is strongly suggested that CTF provide an interface that provides the MAMBA scratch variables assembly by assembly or pin by pin. This will allow the CTF-MAMBA controller in MPACT to provide small amounts of data to the restart file at a time and reduce the total memory used on the master process. The envisioned call graph is outlined below:

1. Restart file queries MPACT MAMBA interface for assembly iasy on master process
2. MPACT MAMBA interface loops over all pins in assembly iasy

3. For each pin, CTF interface requests MAMBA scratch array
4. CTF reduces this data onto the master node and returns to the MPACT interface
5. MPACT interface stores scratch array for entire assembly and returns to restart file
6. Process continues for all assemblies.

Similarly, this process is reversed for a restart or shuffle. The main difference with the shuffle is MPACT will translate the spatial coordinates appropriately and potentially a flag will be passed to CTF to tell MAMBA to account for the outage.

5 Conclusions

In this report, a methodology for modeling CRUD in MPACT is explained and implemented. A uniform CRUD model is used to demonstrate the ability to capture the effects of CRUD in the neutron transport solution. The uniform CRUD model is used to conduct a series of sensitivity studies across a range of different degrees of CRUD deposition and it was determined that the majority of cases a single ring is sufficient to capture the reactivity effects caused by increased neutron absorption and displacement of moderator material. Finally, the coupling of VERA-CS to MAMBA was considered and many options for implementation are highlighted. The suggestion is that CTF control the calls to MAMBA and implement a few additional coupling interfaces to provide input data for the coupling and access the MAMBA solution data. The handling of the MAMBA scratch data needed for the restart must be done very carefully in order to keep the memory footprint of the restart operation manageable. It is highly suggested that the size of this scratch variable be examined to determine if the scope of the data could be reduced. Currently the entire isotopic restart file is approximately 3 GB in size and the storage data requested by MAMBA is 12.4 GB. This will have significant burden to the user if the size of this file is not reduced.

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7 References

1. J. Secker, R. Milanova, Y. Sung, P. Hilton, B. Coulter, K. Belcourt, R. Schmidt, "Coupled ANC/VIPRE/BOA Multi-Physics Results for Watts Bar 1 Cycles 1-3," CASL-2011-0125-000-CI. (2011).
2. B.K. Kendrick, J. Barber, "Initial validation and benchmark study of 3D MAMBA v2.0 against the WALT loop experiment and BOA v3.0". L3.MPO.CRUD.P5.02 (2012).
3. B. Kendrick, D. Walter, B. Collins, V. Petrov, A. Manera, T. Downar, "Proof-of-concept of DeCART/STAR-CCM+/MAMBA Coupled Simulation for the prediction of crud deposition on a fuel pin with grid spacers," L1:CASL.P4.02 (2012).

4. B.T. Nadiga, M.A. Christon, M. Berndt , B.K. Kendrick, “Surface Chemistry Capability in Hydra-TH,” LA-UR 14-27156 (2014).
5. A. T. Godfrey, “VERA Core Physics Benchmark Progression Problem Specifications,” CASL-U-2012-0131-004 (2014).
6. J. Secker. Personal communication (2015).