# VALIDATION OF 3-DIMENSIONAL NEUTRON-TRANSPORT CALCULATIONS OF CANDU REACTIVITY DEVICES

Michaela Ovanes and James V. Donnelly

Atomic Energy of Canada Limited Sheridan Science and Technology Park 2251 Speakman Drive, Mississauga, Ontario, Canada L5K 1B2 Ovanesm@aecl.ca; Donnellyj@aecl.ca

#### ABSTRACT

It is the stated intent within the nuclear industry in Canada that the WIMS-AECL/RFSP suite of codes be adopted as the industry-standard tools (IST) to be used in CANDU<sup>1</sup> reactor-physics analysis. That decision being made, it is therefore essential to represent the reactivity devices in a form that is compatible with the two-group WIMS-AECL-based lattice properties. In a three-dimensional reactor-core model, the reactivity devices are usually represented with incremental cross sections derived through supercell calculations. These incremental cross sections are added to the basic lattice-cell properties to evaluate the effect of the device on neutron-flux distributions and system reactivity. The supercell methodology that has recently been adopted for performing incremental-cross-section calculations for CANDU reactivity devices is based on the DRAGON code. This method uses explicit three-dimensional neutron-transport theory to calculate the macroscopic neutron-flux distribution in and around CANDU reactor fuel channels and reactivity-control devices. The present paper reviews the validation of 3-D DRAGON neutron-transport calculations of CANDU reactivity-device properties against measurements made in two CANDU reactors.

### 1. INTRODUCTION

The full set of nuclear cross sections required to solve the finite-difference neutron-diffusion equation for a CANDU reactor is evaluated by means of a three-step process:

- First, the bare-lattice cross sections are generated for each basic lattice cell in the core, through a cellcode calculation. Since reactivity devices are not present everywhere in the core, they do not affect every lattice cell, and are therefore not included in the cell calculations.
- The second step refers to the representation of reactivity devices, which, in CANDU reactors, are placed vertically or horizontally at some locations in the moderator, interstitially between fuel channels. In a three-dimensional reactor model, the reactivity devices are usually represented with incremental cross sections generated through a supercell calculation.
- In the last step, these incremental cross sections are added to the unperturbed lattice-cell properties to represent the effects of the device on neutron-flux distributions and system reactivity.

<sup>&</sup>lt;sup>1</sup> CANDU® is a registered trademark of Atomic Energy of Canada Limited (AECL)

Until recently, the cell-code POWDERPUFS-V (PPV) [1] has been used to generate the bare lattice-cell properties required for CANDU core simulations with the Reactor Fuelling Simulation Program (RFSP) [2]. The PPV code is a semi-empirical code based on the results of experimental measurements in heavy-water-moderated lattices. However, to overcome these limitations of the PPV code, the PPV-based lattice calculations are now being replaced by WIMS-AECL-based lattice-cell calculations. A two-energy-group option in the RFSP code has been developed and functionally tested, and is now being validated. In this context of migrating to WIMS-AECL [3, 4] as the industry standard code for cell calculations, 2-group device incremental cross sections, compatible with WIMS-AECL lattice-cell cross sections, are required. Current requirements for code validation, as well as the need to analyze sophisticated cell geometries and new reactor designs, have also led to the selection of a more theoretically rigorous code for supercell calculations. Therefore, the diffusion-based MULTICELL code [5], used in the past for conventional supercell calculations, is now being replaced by the transport-based DRAGON code [6] as the industry standard tool for the generation of 2-group device incremental cross sections.

The particular configuration of CANDU reactors, horizontal fuel channels separated by heavy-water moderator and interstitial reactivity control devices, results in a true 3-dimensional (3-D) problem, and the neutronic characteristics of this problem require that the neutron-flux solution be performed in 3-D calculations. DRAGON uses explicit three-dimensional neutron-transport theory to calculate the 3-D neutron-flux distribution in and around CANDU-reactor fuel channels and reactivity-control devices. The application of 3-D neutron-transport calculations in the DRAGON code to this problem has been successfully validated for three types of CANDU reactivity-control devices: light-water-filled liquid zone controllers (LZCs), stainless-steel adjuster rods, and shutoff rods (SORs)/mechanical-control absorbers (MCAs). To qualify the application of DRAGON to CANDU reactivity-device analysis, the calculated reactivity-device properties were compared against reactivity measurements in power reactors. In this document, comparisons are made between calculated device reactivity worths and reactivity measurements performed during commissioning of two CANDU reactors, Pickering-A Unit 4 and Darlington-NGSA Unit 4.

# 2. **REACTIVITY-DEVICE MEASUREMENTS**

In this work, reactivity-device measurements in two different CANDU reactors were analyzed: LZCs and adjuster rods in Pickering-A Unit 4, and SOR and MCA rods in Darlington NGS-A Unit 4. All reactivity measurements were performed during Phase-B commissioning with fresh natural-uranium fuel, at low reactor power. The device-calibration measurements were made by reactivity balance against dissolved neutron poisons in the moderator, and by inter-device reactivity balance. The procedure used to perform calibration tests and the method used to measure the reactivity worth of the three types of control devices discussed here were as follows:

- 1. Batches of moderator poison (gadolinium, boron), designed to add specific "amounts" of negative reactivity, were prepared in advance.
- 2. The Liquid-Zone Controller System worth was determined by observing the change in average zone level (AZL) which results from the addition of these poison batches.
- 3. Other reactivity-device worth is determined by observing the change in AZL that results from device insertion or withdrawal.

*Liquid Zone Controllers*: there are 14 zone controllers in the Pickering-A Unit 4 reactor. Each device consists of a cylindrical compartment containing light water and helium gas, the level of light water being varied under automatic control of the reactor regulating system to implement bulk and spatial control. The calibration of the zone controllers was performed using reactivity balance against pre-weighed

batches of gadolinium which were added to the moderator, and recording the change in average LZC levels at criticality.

*Adjuster Rods*: these devices (6 in the Pickering-A Unit 4 reactor), made of a cylindrical shim rod placed inside a stainless-steel tube, are normally residing in the core. Under normal operation, they may be moved in or out of the reactor core under automatic control of the reactor regulating system to flatten the neutron-flux shape. These devices were calibrated against the LZC system by sequentially or individually withdrawing or inserting adjuster rods, and measuring the change in average LZC levels at criticality.

Shutoff Rods/Mechanical Control Absorbers: 32 SORs are provided in the Darlington NGS-A Unit 4 reactor as part of shutdown system #1, all these rods being fully withdrawn and available out of the core under normal operation, and inserted into the reactor to rapidly reduce core reactivity under accident conditions. Each device is a cylindrical tube, the neutron-absorbent material being a cadmium sheet sandwiched between two concentric stainless-steel tubes. The 4 MCAs, which are provided as part of the reactor regulating system, are physically identical to the SORs, and normally reside out of the core. All these devices were calibrated against the LZC system by individually inserting rods, and measuring the average LZC levels at criticality. During the sequential MCA insertion and withdrawal measurements, initial average LZC fills were adjusted by changing moderator boron concentrations.

In this study, all the adjuster, MCA and SOR calculated reactivity worths are relative to the reactivity worth of the measured changes in zone-controller level. The accuracy of the reactivity measurements would be dependent upon the accuracy of the pre-measured gadolinium batches used to relate zone response to reactivity change. It also depends upon the extent to which the changes in zone level can be accurately measured. Generally, for reactivity changes that correspond to 20% to 40% of AZL change, an uncertainty of about 5% is typically associated with the measurements of zone-controller level changes.

# 3. STANDARD METHOD OF CALCULATING INCREMENTAL CROSS SECTIONS OF CANDU REACTIVITY DEVICES

The DRAGON computer code is a multigroup transport-theory lattice-cell and supercell code that can simulate the neutron-flux distribution inside a unit cell or a fuel assembly in a nuclear reactor. It has been developed and continuously maintained at Institut de Génie Nucléaire, École Polytechnique de Montréal. One of the main advantages that DRAGON offers is the possibility to couple inside a single code detailed multigroup neutron-transport calculations for 2- and 3-dimensional geometries (such as mixed Cartesian and r-q-z geometries) in a collision-probability formalism. Thus, whilst appealing to a completely consistent set of nuclear data, it is possible within DRAGON to perform sophisticated 2-D lattice-cell and 3-D supercell calculations with the required spatial discretization and precision, or few-group calculations in regular production analysis where saving computer time is of prime importance. In this study, DRAGON has been used primarily as a supercell code to calculate the incremental properties representing CANDU reactivity devices.

The neutron-transport calculations were performed using an 89-energy-group ENDF/B-V nuclear-data library. All geometric models were based on the standard 28.575 cm-square unit cell, with the material properties representing natural-uranium fuel and conditions of the Phase B measurements for each of the reactors under study. A typical supercell geometry used in the 3-D DRAGON models is illustrated in Figure 1. The supercell models were all of dimensions 2 lattice pitches x 1 lattice pitch x 1 bundle length (57.150 cm x 28.575 cm x 49.520 cm), which is the normal supercell size given the device arrangement and symmetries in the reactor cores.

The overall calculational strategy for the generation of reactivity-device incremental cross sections can be summarized as follows:

- 1. Two-dimensional (2-D) cluster cell calculations in 89 energy groups
- 2. 89-group macroscopic-cross-section ( $\Sigma_x$ ) computations using the 2-D results;
- 3. Homogenization of fuel-cladding-coolant region without energy condensation;
- 4. Cylindrization of the reactivity device, if necessary;
- 5. Two-bundle-model 3-D supercell calculation with and without the reactivity device; and
- 6. Incremental-cross-sections ( $\Delta \Sigma_r$ ) calculations using the difference between the previous 3-D results.

Following the transport calculation of the spatial flux distribution in Step 5, all cross sections were calculated as 2-energy-group properties, since full-core diffusion calculations are done using two (fast and thermal) energy groups. Finally, a standard flux-volume homogenization technique was performed on each axial plane of the model to generate the region-homogenized incremental properties that will be used to represent the effect of each reactivity device in the reactor core. The region over which the nuclear macroscopic properties are homogenized is defined to be centered on the reactivity device and to extend from the centre of one fuel bundle to the centre of the next fuel bundle along the x axis, as shown in Figure 2. This homogenization scheme (1-LP homogenization over the inner volume of the 2-LP supercell) was selected from the results of a sensitivity analysis considering theoretical rigour, and model preparation and processing effort.

The reactivity-device incremental cross sections, as produced in Step 6, are subsequently used as standard input to the RFSP code to perform 3-D core diffusion calculations. For a given uniform device, a single set of incremental cross sections is assumed to apply to all lattice cells perturbed by the modelled device volume, regardless of position. The region over which the incremental cross sections are applied in 3-D core models is chosen to approximate the spatial extent over which the local perturbation caused by the reactivity device is significant (typically the device length x 1 lattice pitch x 1 bundle length).

#### 4. **RESULTS**

All the reactivity-worth calculations were performed in two-energy-group diffusion-theory simulations using the RFSP code, with DRAGON-generated 2-group incremental cross sections used to represent reactivity devices in the core model. All the lattice-cell calculations for the reference lattices without reactivity-control devices present were performed using the WIMS-AECL code with the 89-energy-group ENDF/B-V nuclear data library.

4.1 Criteria for Comparison with Measurements

The reactivity worth of the LZCs in the Pickering-A Unit 4 reactor was measured by recording the change in the average LZC fills required to balance the addition of pre-weighed amounts of boron dissolved in the moderator. The criterion used to assess the accuracy of calculations, referred to as "simulation error", was computed from the difference between the reactivity changes calculated from changes in moderator boron and changes in LZC fills:

Simulation Error (%) = 
$$100 \times \frac{\mathbf{r}_{LZC} - \mathbf{r}_{Boron}}{\mathbf{r}_{Boron}}$$
 (1)

The reactivity worths of the adjusters in the Pickering-A Unit 4 reactor, as well as the reactivity worth of the SORs and MCA rods in Darlington NGSA Unit 4 reactor, were measured by recording the changes in average LZC fills required to balance changes in rod configuration. In these cases, the error in the simulation of the commissioning tests was computed from the difference between the reactivity changes calculated from changes in device configuration and changes in LZC fills:

Simulation Error (%) = 
$$100 \times \frac{\boldsymbol{r}_{ADJ} - \boldsymbol{r}_{LZC}}{\boldsymbol{r}_{LZC}}$$
 (2)

Note that the method of measurement does not yield information on the absolute reactivity worth of either the zones or the rods, but only on the reactivity balance between those systems. The absolute reactivity worths of devices are available only from calculated reactivity changes corresponding to configuration changes and calculated moderator poison reactivity coefficients.

#### 4.2 Discussion of Results

The simulation results of LZC reactivity-worth measurements with all adjuster rods inserted in-core are presented in Table 1. The corresponding results for LZC measurements with all adjuster rods in an out-of-core configuration are given in Table 2. The LZC reactivity-worth calculated results show good agreement with measurements, yielding an average error of  $-4.2 \pm 5.9\%$  in the configuration with all adjusters inserted, and  $-6.3 \pm 2.6\%$  with the adjusters withdrawn. These two levels of agreement are consistent statistically, and combine to give an average error of  $-5.3 \pm 2.4\%$ .

The simulation results of adjuster-rod reactivity-worth measurements during insertion of individual rods while all other adjusters are kept withdrawn from the core are presented in Table 3. Table 4 presents the simulation results of sequential withdrawal of individual rods, starting from a configuration with all adjuster rods inserted. The agreement in the Pickering analyses between calculated and measured reactivity balance between the light-water-filled liquid-zone compartments and the adjuster rods was -4.5  $\pm$  1.0% in the individual-rod insertions, and -6.8  $\pm$  3.2% in the sequential-withdrawal measurements. These two agreements do not differ statistically, and combine to give an average error of -5.7  $\pm$  1.0%.

The simulation results of the MCA reactivity-worth measurements during absorber sequential insertion tests are presented in Table 5. The simulation results of sequential withdrawal of individual rods beginning from the configuration with all rods inserted are presented in Table 6, and of individual rod insertions with all adjusters out-of-core are presented in Table 7. The agreement in the Darlington analyses between calculated and measured reactivity balance between the light-water-filled liquid zone compartments and the MCAs was  $-1:7 \pm 2:4\%$  during sequential insertion,  $-5.0 \pm 6.5\%$  during sequential MCA withdrawal, and  $-8.4 \pm 4.9\%$  during individual MCA insertions. Note that even though one of the sequential withdrawal measurements (MCA 1) appears to be in error, resulting in an apparently large simulation error (>5 $\sigma$  of the other sequential withdrawal and insertion measurements), it was still considered when calculating the average error. The agreements between sequential MCA insertions and withdrawals are consistent statistically, and combine to give an average of  $-3.4 \pm 2.3\%$ .

The simulation results of SOR reactivity-worth measurements during insertion of individual rods, while all other rods are kept withdrawn from the core, are presented in Table 8. In the analysis of the reactivity worths of SORs during individual rod insertions, the calculations show good agreement with the measurements, with an average error of  $-6.6 \pm 4.2\%$ .

### 5. CONCLUSIONS

The application of 3-D neutron-transport calculations of CANDU reactivity devices with the DRAGON code has been successfully validated against measurements made in the Pickering-A Unit 4 and Darlington-NGSA Unit 4 reactors, for three types of reactivity-control devices: light-water liquid zone-controllers, adjuster rods, and shutoff rods/mechanical-control absorbers.

The general trend for all device-calibration cases was that the calculated device reactivity worth underestimated the calculated worths of measured zone-level changes, or the calculated worths of measured changes in moderator boron in the case of liquid-zone-control calibration. The calculation accuracy obtained for each of the measured devices can be summarized as follows:

- The reactivity worth of the liquid zone controllers was calculated to be on average  $5.3 \pm 2.4\%$  less than the calculated worth of measured changes in moderator boron concentration.
- The reactivity worth of adjuster rods was calculated to be on average  $5.7 \pm 1.0\%$  less than the calculated reactivity worth of measured changes in the average LZC fills.
- The reactivity worth of individual shutoff was calculated to be on average 6.6 ± 4.2% less than the calculated reactivity worth of measured changes in the average LZC fills. Similarly, the reactivity worth of the mechanical-control absorbers was found to be underestimated on average by about -3.4 ± 2.3% relative to the reactivity worth of measured changes in average zone-controller fills.

These levels of agreement are considered to be within an acceptable range for Phase-B commissioning measurements.

# ACKNOWLEDGMENTS

The authors would like to thank the CANDU Owners Group (COG) for financial support. Thanks are also due to G. Marleau and R. Roy from École Polytechnique de Montréal for continuous support with the DRAGON code, and to M.K. O'Neill and F. Dermarkar from Ontario Power Generation Inc. for providing the detailed measurement data of Phase B Commissioning tests.

### REFERENCES

- 1. E.S.Y. Tin and P.C. Loken, "POWDERPUFS-V Physics Manual", TDAI-31, Part1 of 3, 1979 July
- 2. B. Rouben, "Overview of Current RFSP-Code Capabilities for CANDU Core Analysis", Atomic Energy of Canada Limited Report, AECL-11407, 1996.
- 3. R. Askew, F. J. Fayers, and P. B. Kemshell, "A General Description of the Lattice Code WIMS", Journal of the British Nuclear Engineering Society, 5:564-585, 1966.
- 4. J.V. Donnelly, "WIMS-CRNL: A User's Manual for the Chalk River Version of WIMS", Atomic Energy of Canada Limited Report, AECL-8955, 1986 January.
- 5. A.R. Dastur and D. Buss, "MULTICELL a 3-D Program for the Simulation of Reactivity Devices in CANDU Reactors", AECL Report AECL-7544, February 1983.
- 6. G. Marleau, A. Hebert, and R. Roy, "A User Guide for Dragon Version DRAGON\_980911 Release 3.03", Technical Report IGE-174 Revision 4, École Polytechnique de Montréal, 1998 September.

Boron	Calculated	LZC Fill	Calculated LZC	Simulation
Concentration	Boron Reactivity	(%)	Reactivity	Error
(ppm)	Change (mk)		Change (mk)	(%)
9.850	0.00	88.4	0.000	-
9.906	0.39	74.3	0.42	+7.7
9.963	0.79	65.0	0.73	-7.6
10.019	1.18	56.1	1.05	-12.4
10.076	1.58	45.0	1.51	-4.4
10.132	1.97	38.5	1.82	-7.6
10.189	2.36	29.3	2.28	-4.2
10.245	2.75	21.0	2.73	-0.7
Average				$-4.2 \pm 5.9$ %

Table 1LZC Reactivity Worth with Adjusters In-Core

Table 2LZC Reactivity Worth with Adjusters Out-of-Core

Boron	Calculated	LZC Fill	Calculated LZC	Simulation
Concentration	Boron Reactivity	(%)	Reactivity	Error
(ppm)	Change (mk)		Change (mk)	(%)
11.261	0.00	91.4	0.00	-
11.317	0.39	79.4	0.36	-7.7
11.374	0.79	68.4	0.71	-10.1
11.430	1.18	56.8	1.12	-5.1
11.487	1.57	48.4	1.44	-8.3
11.543	1.97	38.5	1.85	-6.1
11.599	2.36	30.0	2.24	-5.1
11.656	2.75	19.9	2.71	-1.5
Average				-6.3 ± 2.6 %

Table 3Adjuster Reactivity Worths(Sequential Withdrawal Starting with Adjuster Out-Of-Core)

Adjuster Rod	Average 7 ADJ out Initial (%)	Zone Level ADJ in Final (%)	Calculated LZC Reactivity Worth (mk)	Calculated ADJ Reactivity Worth (mk)	Simulation Error (%)
AA-7	73.5	35.5	1.43	-1.39	-2.8
AA-12	73.7	34.5	1.48	-1.40	-5.4
AA-9	73.5	34.6	1.47	-1.40	-4.8
AA-10	73.5	35.1	1.45	-1.39	-4.1
AA-8	73.6	20.2	2.26	-2.13	-5.8
AA-11	73.3	20.1	2.22	-2.13	-4.1
Average					-4.5 ± 1.0 %

Table 4Adjuster Reactivity Worths(Sequential Withdrawal Starting with Adjuster In-Core)

Adjuster Rod	Average 7 ADJ out Initial (%)	Zone Level ADJ in Final (%)	Calculated LZC Reactivity Worth (mk)	Calculated ADJ Reactivity Worth (mk)	Simulation Error (%)
AA-7	21.0	46.8	-1.30	1.12	-13.8
AA-12	31.3	54.9	-1.09	1.02	-6.4
AA-9	29.6	60.3	-1.41	1.35	-4.3
AA-10	30.5	58.1	-1.28	1.20	-6.3
AA-8	29.3	71.9	-1.78	1.68	-5.6
AA-11	20.9	73.0	-2.10	2.01	-4.3
Average					-6.8 ± 3.2 %

Table 5	
Mechanical Control Absorber Reactivity Wo	rths
(Sequential MCA Insertion)	

MCA Rod	Average 7 MCA out Initial (%)	Zone Level MCA in Final (%)	Calculated LZC Reactivity Worth (mk)	Calculated MCA Reactivity Worth (mk)	Simulation Error (%)
1	69.8	43.0	1.77	-1.72	-2.8
4	70.8	34.0	2.39	-2.37	-0.8
3	71.3	41.3	1.92	-1.95	+1.6
2	73.0	19.0	3.24	-3.08	-4.9
Average					-1.7 ± 2.4 %

Table 6	
Mechanical Control Absorber Reactivity	Worths
(Sequential MCA Withdrawal)	

MCA Rod	Average Z MCA out Initial (%)	Zone Level MCA in Final (%)	Calculated LZC Reactivity Worth (mk)	Calculated MCA Reactivity Worth (mk)	Simulation Error (%)
2	19.0	70.5	-3.31	3.24	-2.1
3	32.50	60.4	-1.94	1.93	-0.5
4	25.5	60.4	-2.49	2.46	-1.2
1	23.7	51.7	-2.09	1.75	-16.2
Average					$-5.0 \pm 6.5$ %

Table 7 Mechanical Control Absorber Reactivity Worths (Individual MCA Insertion)

MCA Rod	Average Z MCA out Initial (%)	Cone Level MCA in Final (%)	Calculated LZC Reactivity Worth (mk)	Calculated MCA Reactivity Worth (mk)	Simulation Error (%)
1	64.8	31.2	2.05	-1.89	-7.8
2	64.9	27.9	2.01	-2.02	-0.5
3	65.1	27.8	2.32	-2.04	-12.1
4	64.1	29.2	2.16	-1.88	-13.0
Average					-8.4 ± 4.9 %

Shutoff	Average	Zono Loval	Coloulated J 7C	Coloulated SOD	Cimulation
Pod	Average Z	MCA in	Calculated LZC Ponctivity Worth	Calculated SOR	Error
Kou	Initial (%)	Final (%)	(mk)	(mk)	(%)
	finitial (%)	1-111al (70)	(IIIK)	(IIIK)	(70)
1	63.7	54.5	0.63	-0.59	-6.3
2	63.7	44.2	1.36	-1.31	-3.7
3	63.7	43.2	1.42	-1.34	-5.6
4	63.7	53.5	0.68	-0.60	-11.8
5	63.7	46.5	1.17	-1.07	-8.5
6	63.7	38.0	1.73	-1.61	-6.9
7	63.7	45.2	1.26	-1.10	-12.7
8	63.7	48.6	1.04	-0.94	-9.6
9	63.7	48.0	1.08	-0.95	-12.0
10	63.7	45.6	1.30	-1.22	-6.2
11	63.7	40.2	1.71	-1.61	-5.8
12	63.7	37.0	1.96	-1.93	-1.5
13	63.7	34.0	2.13	-2.16	+1.4
14	63.7	36.0	2.02	-1.95	-3.5
15	63.7	39.1	1.77	-1.60	-9.6
16	63.7	44.3	1.39	-1.21	-12.9
17	63.4	44.8	1.35	-1.23	-8.9
18	63.0	39.8	1.69	-1.63	-3.6
19	63.0	36.0	1.99	-1.98	-0.5
20	62.8	33.7	2.11	-2.17	+2.8
21	62.8	36.2	1.94	-1.91	-1.5
22	63.2	39.4	1.72	-1.58	-8.1
23	63.0	44.1	1.36	-1.20	-11.7
24	63.2	47.2	1.11	-0.97	-12.6
25	62.8	47.8	1.04	-0.93	-10.6
26	62.8	45.4	1.21	-1.12	-7.4
27	62.7	37.5	1.69	-1.63	-3.6
28	63.0	45.4	1.20	-1.06	-11.7
29	63.2	53.6	0.66	-0.62	-6.1
30	63.0	43.0	1.40	-1.35	-3.6
31	63.0	43.5	1.36	-1.31	-3.7
32	63.0	53.8	0.62	-0.58	-6.5
Average					-6.6 ± 4.2 %

# Table 8 Shutoff-Rod Reactivity Worth (Individual SOR Insertion)



Figure 1 Typical Supercell Model in DRAGON

Single-Volume Homogenization over 1-LP Supercell (Homogenization on the Inner Volume of the 2 LP Supercell)

\*Note: shaded areas represent the volumes used in the homogenization process