## **SDS-2 Modelling with DRAG SHELL**

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#### **Abstract**

For SDS2 physics modelling, Ontario Hydro, "now Ontario Power Generation" introduced an automated methodology driven by a shell script named SDS2-SHELL, which uses the supercell code MULTICELL<sup>[1]</sup> and the lattice code POWDERPUFS-V<sup>[2]</sup>, in order to provide appropriate incremental cross sections corresponding to various stages of poison injection in the moderator. With the current move to newer physics tools, RFSP-IST<sup>[3]</sup> is now required to have the capability to perform SDS-2 analysis in the full-two-energy-group methodology. In order to achieve this functionality, a new shell script, DRAG\_SHELL, which uses the supercell code DRAGON<sup>[4]</sup> and the lattice code WIMS-IST<sup>[5]</sup>, was developed. The new DRAG\_SHELL methodology has been automated using a UNIX Korn shell script. The execution of the suite of codes and the manipulation of the huge input and output data required for SDS-2 simulation is achieved by using intuitive, English language keywords. Some of the features of DRAG\_SHELL include maintaining consistency of code-to-code data transfer and the standardization of input formats.

## Introduction

Shutdown system number 2 (SDS-2) is one of the two independent shutdown systems utilized in CANDU<sup>®</sup> reactors. During a postulated loss-of-coolant accident (LOCA), SDS-2 can rapidly shut down the reactor by injecting liquid poison at high pressure into the moderator through six horizontal nozzles. The liquid poison, in the form of gadolinium nitrate dissolved in  $D_2O$ , is injected at high pressure into the moderator through holes in the nozzles, initially as jets, which rapidly merge into a curtain. LOCA analysis involving the dynamics of liquid-poison injection is extremely complicated and very difficult to model. The main difficulty is the representation of the propagation of the poison curtain in the moderator. The calculation of appropriate incremental cross sections to represent the poison involves intensive modelling and data manipulation.

# **Physics Modelling**

The physics modelling of SDS-2 accounts for the major phenomena that occur, by combining the effects of both the moderator hydraulics and the neutronics. The moderator hydraulics must provide realistic modelling of the poison volumes and of the time of entry of the poison fluid into the reactor, as well as propagation of the poison into the moderator after emission from the nozzle. The neutronics must provide an accurate

<sup>+</sup> This work was funded by the CANDU Owners Group CANDU<sup>®</sup> is a registered trademark of AECL

evaluation of the reactivity worth of varying volumes and geometries of poisoned moderator fluid for a range of poison concentrations, in order to simulate the reactivity effect of the injected poison. The first type of data is generated by the moderator hydraulics code ALITRIG. The neutronics data is generated for a number of standard geometries and concentrations using the lattice cell code DRAGON. More specifically, the liquid poison is emitted from a number of horizontal pipes or nozzles within the reactor core. As the poison moves away from the nozzle, it expands in a conical shape. The neutronics calculation must simulate the variety of geometries that ensue, i.e., the poison inside the nozzle before emission, and poison jets exiting the pipe at several potential orientations: horizontally, vertically or at 45 degrees to the horizontal. In the modelling used here, the emitted jet evolves as an expanding cone, which is represented by parallelepipeds of three different thicknesses: 3.5, 4 and 4.5 cm. Table 1 shows the poison concentrations considered in our calculations. The choice of concentrations used in the generation of cross sections is arbitrary; however it is intended to provide a range of concentration values with which to interpolate, in order to find the cross section for jet geometries and concentrations that occur during the injection of poison.

Table 2 shows the composition of the poison<sup>[6]</sup>.

### **CODE DESCRIPTIONS**

Figure 1 shows a schematic diagram of the codes and data flow managed by DRAG\_SHELL. DEMON is used to generate the geometric mesh structures for each corresponding nozzle and jet geometry. Following the execution of DEMON, the next step involves running DRAGON, which uses three-dimensional mesh structures (generated by DEMON) to produce the cell-average macroscopic cross section for all jet-nozzle combinations (Figures 2 to 7) with various poison concentrations required by INCON. For the modelling of SDS-2, the following nozzle combinations are used:

- 1. Nozzle only, with poison inside (Figures 2).
- 2. Jets only, emitted either vertically or horizontally (Figure 3 and 4 respectively).
- 3. Jets only, emitted at 45 degrees to the horizontal (Figure 5)
- 4. Vertical or horizontal jets, attached to nozzle (Figure 6)
- 5. 45-degree jets, attached to a nozzle (Figure 7)

Figure 8 shows an Idealized view of the poison injection region for 45 degree jets.

Following the DRAGON calculation, DRAG\_COLLATE is executed. This code is used to assemble all the data from DRAGON into a single file that can be accessed by INCON. INCON reads the collated data from DRAGON and uses the jet length and injected poison volume at each time step calculated by ALITRIG to tabulate the cross sections as a function of jet length and poison concentration by using Lagrange polynomial interpolation. Here, ALITRIG is the moderator hydraulics code that is used to simulate injection into the reactor from the poison-filled tanks driven by a high-pressure gas tank. The execution of POISON follows INCON. POISON reads the input data from INCON and then prorates the incremental cross sections, based on the jet length and poison concentration at various times, in order to represent an appropriate three-dimensional poison cell as a function of space and time for each nozzle. These

incremental cross sections are then used in the kinetics calculation within the \*CERBERUS module of RFSP-IST.

The descriptions of the programs managed by DRAG\_SHELL script are given below.

### DEMON

The DRAGON code, which is used to calculate cell-average macroscopic cross sections in two neutron-energy groups, uses the three-dimensional rectangular (xyz) mesh generated by DEMON. The actual geometries of the physical system are circular-cylindrical. To describe circular cylinders in a rectangular mesh, certain geometry transformations are required. DEMON generates a three-dimensional rectangular (xyz) mesh for every combination of geometry and poison-jet thickness.

The following conservation rules are applied during the geometry transformations for each of the above geometries:

- 1. Conserve the surface area of the fuel.
- 2. Conserve the surface area of the poison jet.
- 3. Conserve the surface area of the poison in the nozzle
- 4. Conserve the moderator volume.

Following the execution of DEMON, the next step involves running DRAGON to produce the average macroscopic cross sections in two energy groups for all jet-nozzle combinations with various poison concentrations. In fact, DRAG\_SHELL uses the output from DEMON (the three-dimensional mesh structures) and automatically generates the required DRAGON input files, named DRAG\_geometry, for each combination of geometry and poison. This represents about 150 distinct DRAGON files. Each file is assigned a name that reflects the geometry for which it was created. For example, the file DRAG\_jt45t1 refers to a detached jet emitted at 45 degrees to the horizontal with thickness t1. The emitted jets evolve as expanding cones that are represented by parallelepipeds of three different thicknesses.

## DRAGON

The DRAGON neutron-transport code was designed for general geometry and can analyse both CANDU clusters and PWR assemblies in 2-D. The code can also carry out 3-D supercell transport calculations with the same group structure as the 2-D analysis to obtain few-group properties for supercells containing in-core reactivity devices. DRAGON contains three different modules for self-shielding calculations and transport calculations. In this study, the EXCELT and EXCELL modules (collision probability method for general 2-D and 3-D geometry) were used for CANDU 2-D cell and 3-D supercell calculations, respectively. The EXCELL module, which integrates the features of previous EXCELT and ASM (computation of collision probability matrices) modules, enables users to do fine-mesh calculations in 3-D domains without any limitation on the size of the tracking file. A brief description of DRAGON modelling is given here. Ref.

[7] provides more detail on CANDU 2-D cell calculations and 3-D supercell calculations with DRAGON.

DRAGON was selected as the standard 3-D supercell code for CANDU analysis based on the following considerations:

- the DRAGON multigroup neutron-transport method is theoretically rigorous, is relatively straightforward, and is consistent with the WIMS-IST lattice calculations;
- it has an exact or nearly exact geometrical representation of the devices and the fuel channels; and
- the results of various benchmark comparison are all within the acceptable ranges.

All the cell and the supercell calculations reported in this study were performed using DRAGON code version 3.03a with the 89-group ENDF/B-V library. The current standard version of WIMS-IST was used here only for 2-D-cell depletion calculations, to generate the reference fuel composition at the nominal mid-burnup.

A standard 2-D CANDU-6 cell transformed to cylindrical geometry has been defined and used as the basis for all supercell calculations. To generate supercell properties, 2-D calculations are performed. Properties are homogenized in three regions: the fuel area, calandria and pressure tubes, and the moderator region. No energy condensation is performed. The multigroup transport calculation is performed with the 2-D collision-probability module (EXCELT) in DRAGON, using the B<sub>1</sub> homogeneous leakage method<sup>[4]</sup>. The isotropic reflective tracking was used with 29 angles and 20 lines/cm. Table 3 shows a summary of reactor nominal conditions used in these simulation.

Following the DRAGON 2-D CANDU lattice cell calculations, the 3-D supercell calculations were carried out in DRAGON with the same 89-group structure as used in the 2-D cell calculations. Two types of DRAGON calculations are performed; a reference cell with no reactivity device or poison, and a "device-inserted" cell. The reference cell and the "device-inserted" cell depend on the geometry used:

- 1. Case 1: for jets only, emitted vertically, horizontally or at 45 degrees to the horizontal (referred to as detached). The reference cell consists of a number of homogenized regions: the moderator region, the fuel bundle, and the surrounding annulus, which consists of the pressure tube, gas gap and calandria tube. In this case, the "device-inserted" cell also contains a poison jet.
- 2. Case 2: for vertical, horizontal and 45-degree jets (referred to as attached to a nozzle). The reference cell contains, in addition to the homogenized regions (described above), a nozzle with no poison inside. In this case, the "device-inserted" cell also contains a nozzle with poison inside and a poison jet.
- 3. Case 3: for a nozzle only. The reference cell is the same as in case 2. The "device-inserted" cell contains a poison-filled nozzle.

Tracking was performed with the EXCELL module and the isotropic reflection option. The transport equation was solved in the same way as in the cell calculations, using the  $B_1$  homogeneous leakage method. Homogenization and condensation were performed by weighting cross sections using the 89-group flux spectrum with an energy cut-off between the two groups at 0.625 eV. Figures 2 to 7 show the geometries used by

DRAGON for supercell calculation. For simplification purposes only presenting 1/8 of the supercells are presented. In these Figures, LP and BL refer to the bundle length and the lattice pitch respectively. Table 4 shows the composition and the dimension of the nozzle.

## COLLATE DRAGON

This code consists of a set of Unix commands that assemble all the data files from DRAGON into a single file, which can then be accessed by INCON. This collated cross-section file for various jet and nozzle conditions is to be used as an input to INCON.

### **INCON**

The execution of INCON follows that of COLLATE\_DRAGON. INCON reads the collated cross-section data from DRAGON, and uses the jet length and injected poison volume calculated at each time step by ALITRIG to tabulate the cross sections as functions of jet length and poison concentration.

### **POISON**

POISON is a three-dimensional code; it reads the input data from INCON and then prorates the incremental cross sections, based on the jet length and poison concentration at various times, in order to represent an appropriate three-dimensional poison cell. These incremental cross sections are to be used in the kinetics analysis performed by the \*CERBERUS module of RFSP-IST.

## **Results of Transients**

A coupled neutronics/thermahydraulics simulation of transients following a hypothetical large LOCA initiated from a nominal flux shape and terminated by SDS-2 action was carried out. In the LOCA analysis, one of the six poison injection nozzles was assumed to be non-operational upon actuation of SDS-2. The selection of the non-operational nozzle was based on the criterion that the remaining nozzles constitute the least effective set of five nozzles.

All simulations were done in three spatial-time dimensions, with RFSP-IST coupled to the thermalhydraulics code CATHENA. The two codes were coupled in the sense that neutronics and thermalhydraulics equations were solved alternately for the sequence of time steps. At each step, the coolant density, coolant-temperature and fuel-temperature distributions calculated with CATHENA were input to the \*CERBERUS module within RFSP-IST, along with poison incremental cross sections calculated separately (using DRAG\_SHELL), in order to calculate the three-dimensional flux and power distributions.

The SDS-2 simulations are performed with DRAGON using mid-burnup fuel with a composition generated by WIMS-IST. Figure 9 shows the system reactivity as a function of time. Poison entered the core at 1.0586 s after the break. An SDS-2 simulation using the older SDS2\_SHELL methodology was carried out for a LOCA in the CANDU-6 equilibrium core. The results obtained were compared to those obtained here with the

DRAG\_SHELL methodology. Figure 9 shows that the initial reactivity is very similar, but the asymptotic reactivity calculated with DRAG\_SHELL is more negative, by about 8 mk. Figures 10 and 11 show the relative core power and hot bundle relative power transients. Although the asymptotic reactivity is slightly different, the powers are almost the same.

#### CONCLUSION

The aim of this work was to develop a methodology for modelling and analysing the action of SDS-2 in two neutron-energy-groups. This has been achieved by developing a new script, DRAG\_SHELL, which executes under the management of a UNIX-based shell. This configuration permits easy communication among the various parts of the script. DRAG\_SHELL uses a database of incremental cross sections calculated in 2 energy groups with DRAGON, based on the jet length and poison concentration at various times in the postulated transient. This database of cross sections is then used in the kinetics calculations performed with the \*CERBERUS module of RFSP-IST.

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Table 1: Poison (gadolinium nitrate) concentration for each jet and thickness

Thickness 1	Thickness 2	Thickness 3	Thickness 1	Thickness 2	Thickness3	
(3.5 cm)	(4.0  cm)	(4.5 cm)	(3.5  cm)	(4.0  cm)	(4.5 cm)	
Jet only, emitted at 45 degrees,			Jet only, emitted at 45 degrees attached to a			Jet only, 0 and
in ppm			nozzle, in ppm		90 degrees, in	
						ppm
0.00	0.00	0.00	0.00	0.00	0.00	0.00
187.88	207.72	226.32	195.92	216.76	236.32	160.00
563.64	623.16	678.96	587.76	650.28	708.96	480.00
751.52	830.88	905.28	783.68	867.04	945.28	640.00
939.40	1083.60	1131.60	979.60	1083.80	1181.60	800.00
1127.20	1246.30	1357.90	1175.50	1300.50	1417.90	960.00
1503.00	1661.70	1810.50	1567.30	1734.00	1890.50	1280.00
2254.50	2492.60	2715.80	2351.00	2601.10	2835.80	1920.00
3381.80	3738.90	4073.70	3526.50	3901.60	4253.70	2880.00
4697.00	5193.00	5658.00	4898.00	5419.00	5908.00	4000.00

Table 2: Composition of the Poison (gadolinium nitrate)

Isotope	wt %
Gd	0.3481152
N	0.0931263
0	0.5321507
Н	0.0266075

Table 3: Summary of Reactor Nominal Conditions

Fuel Density (g/cm <sup>3</sup> )	10. 39475
Fuel Temperature (K)	941.3
Specific Power (kW/kgU)	31.9713
Coolant Density (g/cm <sup>3</sup> )	0.81790
Coolant Temperature (K)	561.66
Coolant Purity (at %)	99.00
Moderator Density (g/cm <sup>3</sup> )	1.08699
Moderator Temperature (K)	339.16
Moderator Purity (at %)	99.855
Moderator Natural Boron (ppm)	0.00

Table 4: Composition and dimension of the nozzle

	Element	Wt %
	Zr	99.823
	Fe	0.070
	Cr	0.050
	Ni	0.030
	C	0.027
	Density	6.504 (g/cm <sup>3</sup> )
Nozzle Radius		2.8732 cm
Poison Area Radius		2.5400 cm

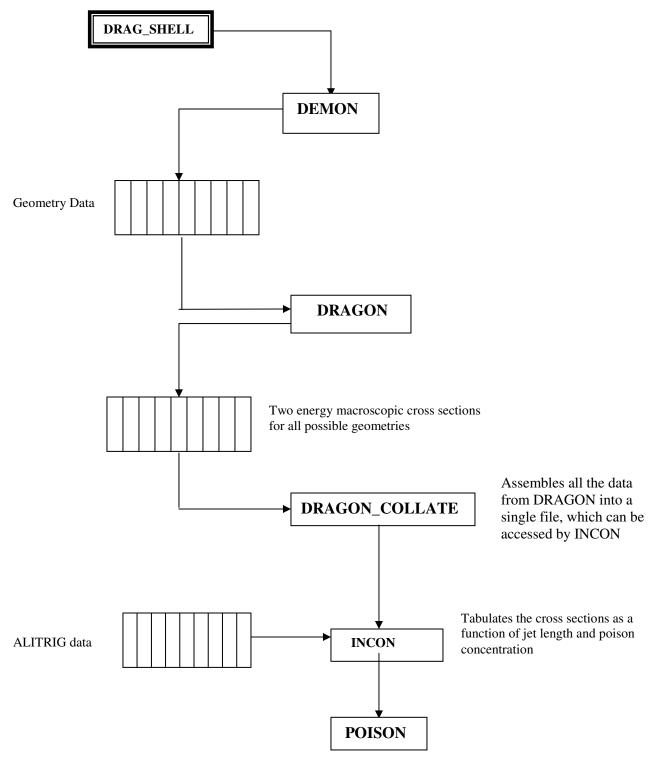
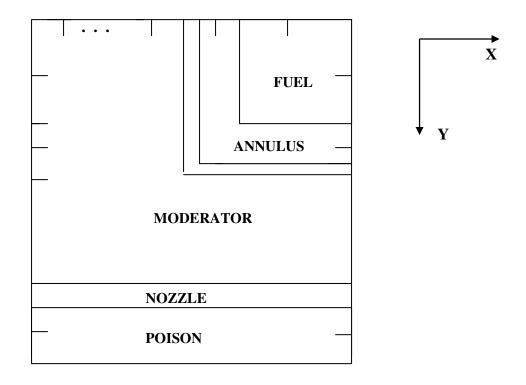


Figure 1: Schematic Diagram of the Codes and Data Flows Managed by DRAG\_SHELL



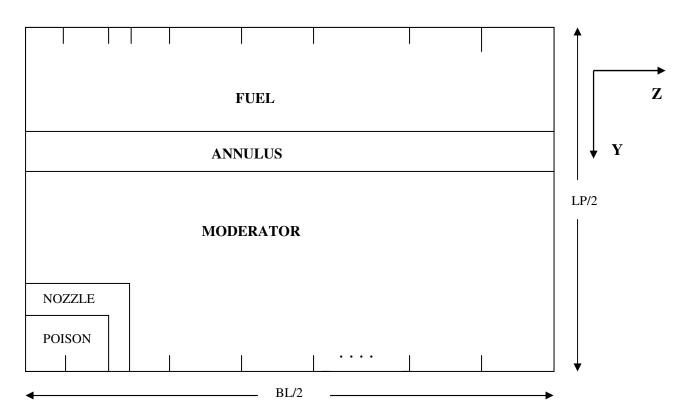


Figure 2: Model for Nozzle Only

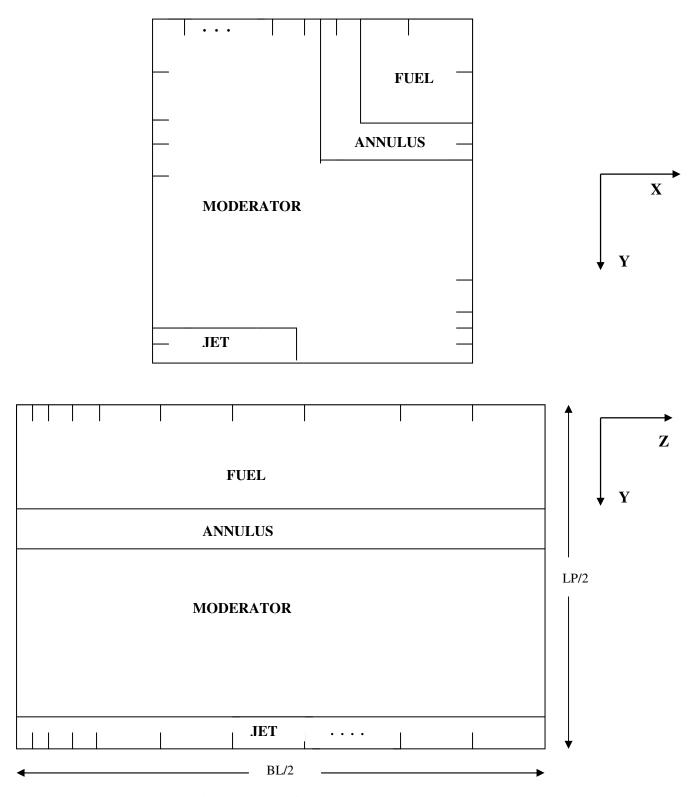


Figure 3: Model for Jets only at 0 Degrees

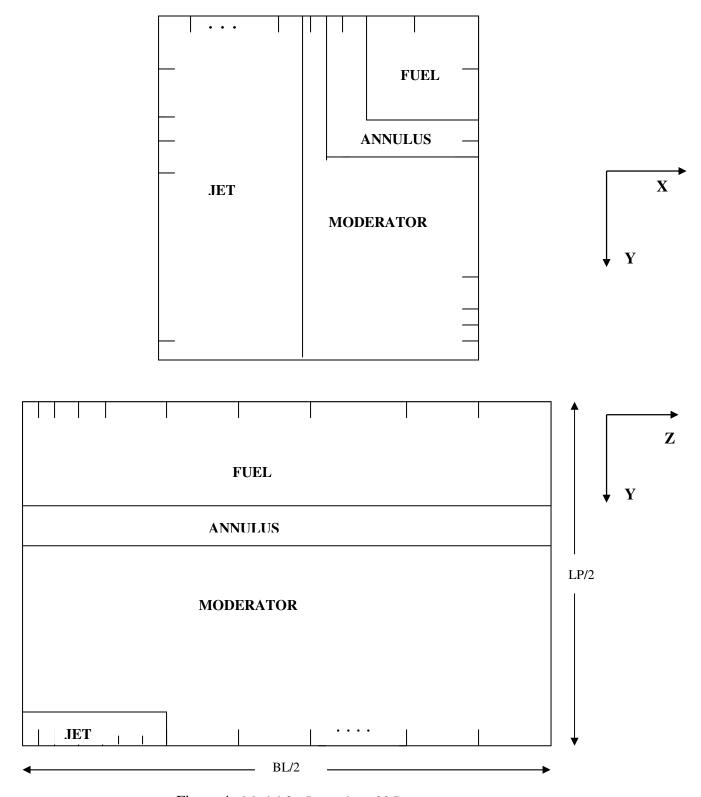
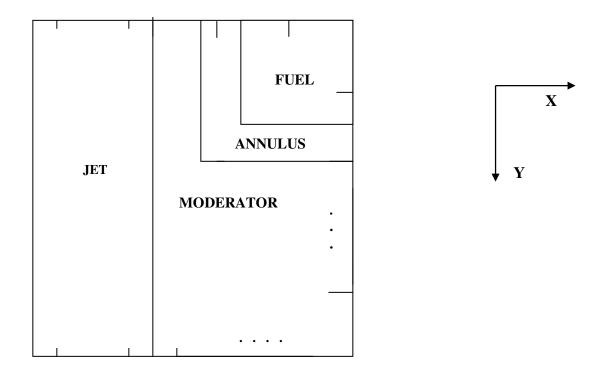


Figure 4: Model for Jets only at 90 Degrees



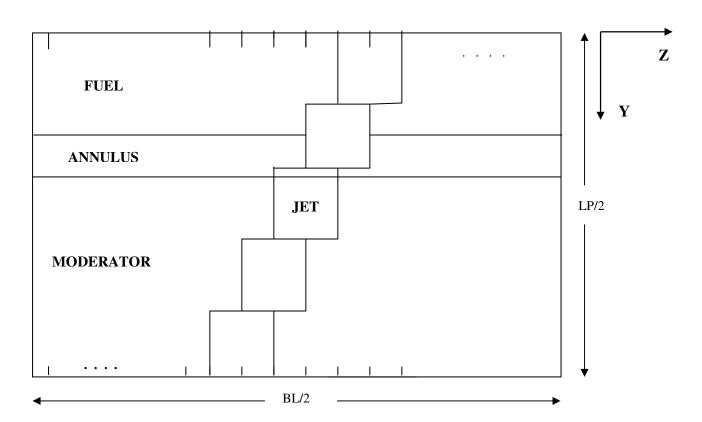
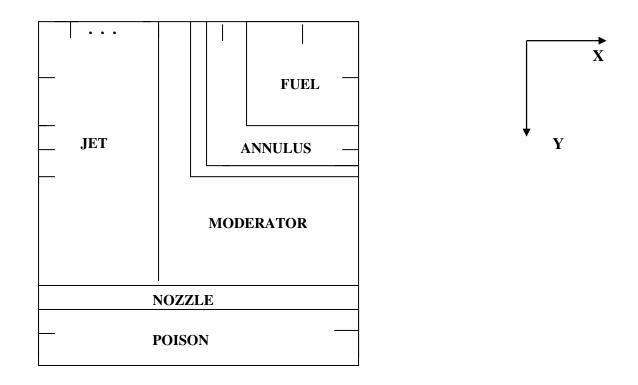


Figure 5: Model for Jets Only at 45 degrees



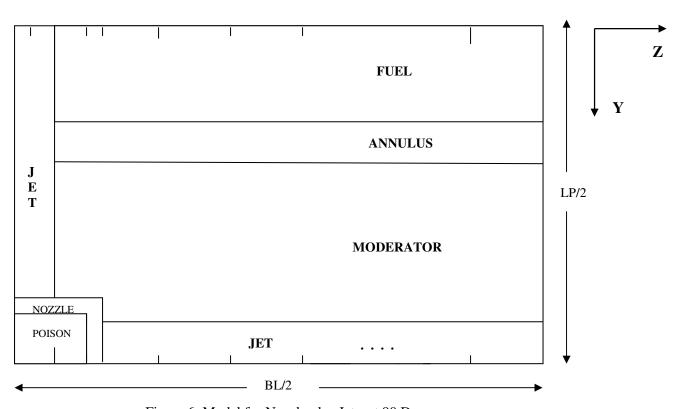
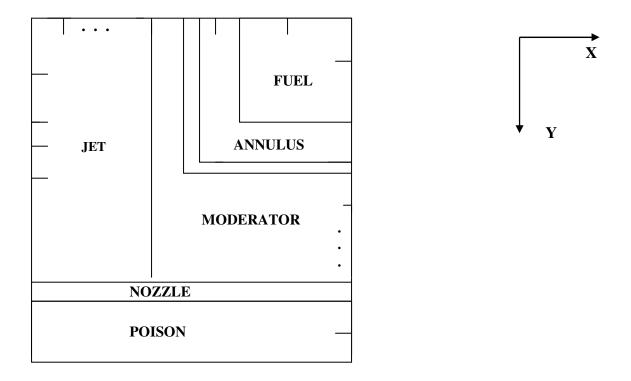


Figure 6: Model for Nozzle plus Jets, at 90 Degrees



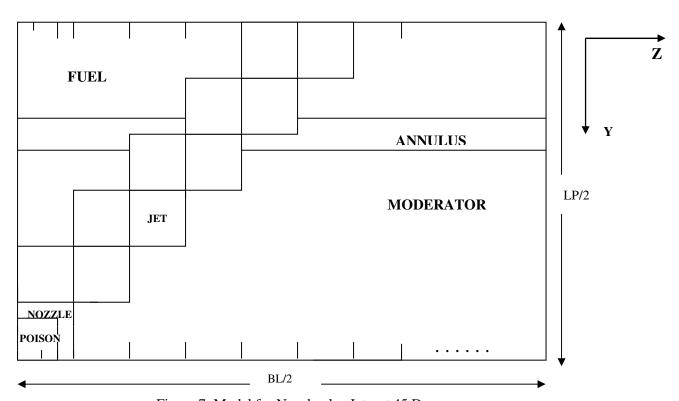


Figure 7: Model for Nozzle plus Jets, at 45 Degrees

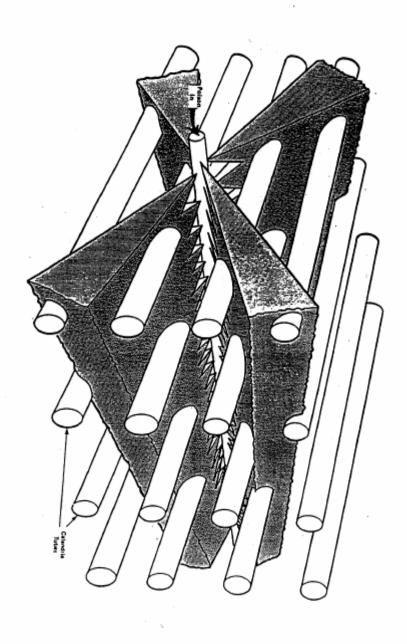


Figure 8: An Idealized View of the Poison Injection Region for 45 Degree Jets

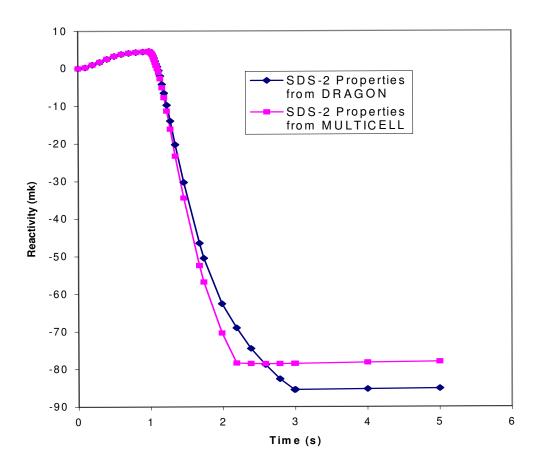


Figure 9: Reactivity Transient vs. Time

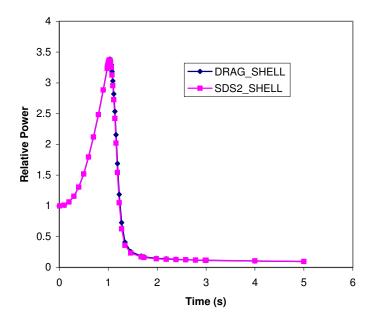


Figure 10: Relative Core Power vs. Time

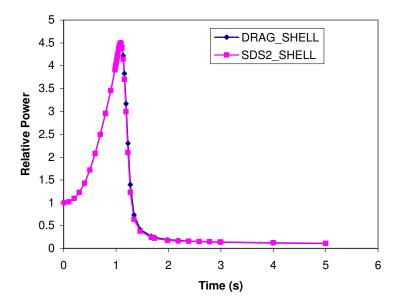


Figure 11: Hot Bundle Relative Power Transients