GOTHIC-IST MODEL OF ISP-47 PHASE B MISTRA EXPERIMENT

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ABSTRACT

International Standard Problem 47 examined the ability of computer codes to predict local gas distributions during experiments simulating Loss of Coolant Accidents with Loss of Emergency Core Coolant (LOCA/LOECC) or Pressurized Water Reactor severe accident scenarios that involve hydrogen release to containment. It involved three experimental test facilities (TOSQAN, MISTRA and ThAI) located in France and Germany. This report documents AECL's GOTHIC-IST 6.1bp2 model of Phase B of the MISTRA experiment with steam condensation in an air-helium atmosphere. The GOTHIC-IST model used to model the TOSQAN test (open simulation) was scaled up to model the MISTRA test (blind simulation). The GOTHIC-IST results are in good agreement with the MISTRA results, except for some anomalies in the experimental results.

1. INTRODUCTION

The goal of the International Standard Problem 47 (ISP-47) is to evaluate the capabilities of CFD and lumped parameter containment thermalhydraulics codes to predict hydrogen distribution under severe accident conditions. As well, ISP-47 seeks to assess the capability of CFD codes to take into account a change in scale.

ISP-47 was split into two steps. The first step was with simple geometries using the TOSQAN and MISTRA facilities. The second step was with a more complex and realistic compartmented geometry using the ThAI facility. The first step of ISP-47 was further broken down into two phases. Phase A dealt with steam-air mixtures; Phase B dealt with steam-air-helium mixtures.

TOSQAN was an open simulation with the experimental results available to the modellers. This allowed the modellers to "tune" their numerical model to obtain an appropriate match with the experiment. MISTRA was a blind simulation and the modellers were to scale up their TOSQAN model to simulate the MISTRA experiment.

Atomic Energy of Canada Limited (AECL) participated in ISP-47 and used GOTHIC-IST 6.1bp2 to model the experiments (unless otherwise specified, GOTHIC will mean GOTHIC-IST 6.1bp2). This report documents the work done by AECL to model the MISTRA experiment in ISP-47 Step 1 Phase B.

2. THE GOTHIC CODE

GOTHIC is a general-purpose thermalhydraulic computer program. It can be used for design, safety and licensing, and operating analysis of nuclear containments and other confinements [1-3]. It is used to calculate the thermalhydraulic response of a reactor building modelled as a collection of inter-connected volumes. Each room can be treated as a lumped parameter or subdivided into a one-, two- or three-dimensional Cartesian mesh.

Model response is determined by solving a combination of mass, momentum and energy conservation equations for three phases: vapour, liquid and droplets, and by solving closure relations for interface mass, energy and momentum transfer. Each phase may have different pressures, velocities, and temperatures. Turbulence in the liquid or vapour phase can be modeled with one of two turbulence models; mixing length and a standard k-ε model (a turbulence model that solves two additional transport equations for turbulent kinetic energy, k, and its dissipation rate, ε).

3. MISTRA EXPERIMENT

Figure 1 shows a cutaway and cross-sectional view of the MISTRA facility. It has an internal free volume of 99.5 m^3 (4.25 m internal diameter, 7.38 m height). It comprises an insulated (20 cm of rock wool) stainless steel containment vessel with three internal stainless steel condensers near its outer walls. There are two injection lines. The main line (upward vertical injection of steam and helium) is axially centred, with an injection diameter of 0.2 m and an upper axial position of 1.295 m. A diffusion cone, designed for gas injection and steam/helium mixing, ensures a flat velocity profile at the injection nozzle. The second injection line is used for containment wall heating with steam.

Table 1 shows the steam and helium injection conditions for phase A and B. Phase A deals with steam condensation in an air environment. Helium is added in Phase B and steam condensation occurs in an air-helium atmosphere. Steady state conditions are reached at the end of each phase. This report is mainly interested with Phase B, but Phase A must be solved to obtain the starting conditions to model Phase B.

One of the objectives of ISP-47 is to test a code's ability to take into account the change in scale (scale the cells to match the increase in volume being modelled, keeping the total number of cells similar). The geometry of the MISTRA facility is similar to that of TOSQAN, with the MISTRA being much larger but with a lower aspect ratio (TOSQAN has an internal free volume of 7.0 m^3, 4 m high and 1.5 m inside diameter), allowing the assessment of code scalability. The experimenters proposed that the participants use the open TOSQAN test to setup their computer models, then scale the model upwards to model the much larger blind simulation of the MISTRA test, using essentially the same number of computational cells.

4. GOTHIC MODEL

The objective of this exercise was to determine GOTHIC's ability to model the following phenomena:

- Multi-component gas compression/decompression, in different dynamics of compression (low and high slope of pressure evolution)
- Jet-plume gas interaction/entrainment, with a typical jet configuration (high steam injection mass flow rate) and a typical plume configuration (lower steam mass flow rate)
- Flows under natural convection, with a part of the test at very low gas velocities in the vessel (close to zero) and other parts of the test with higher velocities
- Heat and mass transfer on the wall for two levels of condensation flux (lower and higher mass flux)
- Flows of three-component gas mixture (helium-air-steam)
- Buoyancy and wall interaction

and to assess the code's ability to scale up to larger sized experiments.

The results were generated using Intel Pentium 4, 1.7 GHz, computers with 256 MB of RAM (RAMBUS PC800). The operating system was Red Hat LINUX 7.1 (kernel 2.4.2-2). GOTHIC was compiled using the GNU C/C++ compiler (version gcc-2.96) with level 1 optimization.

The nodalization of the MISTRA facility, shown in Figure 2, is scaled up from the grid used to successfully model the TOSQAN experiment. The blue shaded region represents the condensers. The bottom right corner of the vessel is blocked off to simulate the curvature of the actual vessel walls and to ensure that there is 99.5 m^3 of vapour space within the model. The GOTHIC model of the MISTRA test employs a non-uniform, expanding-width, 2D Cartesian mesh (approximation of polar coordinates using GOTHIC's Cartesian grid, shown in Figure 3).

The exact initial conditions at the start of Phase A are not known since the pre-heating and cooling phases are not modelled. This is not a problem since the test is run to steady state at the end of Phase A (which become the starting conditions for phase B), but the mass of air at the start must be 118 kg (consistent with the mass of air at the start of the pre-heat phase). Selecting suitable initial conditions of 115°C and 3 bars require an initial relative humidity of 99.307% to achieve the correct initial air mass of 118 kg. The steam and helium injection temperatures and flow rates are shown in Table 1. The condenser surface temperature was set at 115°C for the entire transient. A total of 18.5 kg of helium was injected over a 1740-second period.

Heat transfer from the outside vessel surface was modelled with a heat transfer coefficient of $h = 4.1$ W/m^2•K and an ambient temperature of $T = 20^o$C. The heat transfer coefficient was obtained from a parametric study to result in parasitic condensation being 13.7% of the steam injection rate, as was reported in the MISTRA experiment. The parasitic condensation is calculated as the total condensation occurring on the ceiling, dead space behind the condensers and on the floor.

The given steam injection conditions can lead to an undesirable situation where the steam is injected at a temperature that is lower than the local saturation temperature, which would be contrary to the experimental specification of saturated or slightly superheated steam injection. To prevent this situation, the steam injection temperature in the GOTHIC model was set to as either the specified temperature or 0.5°C higher than the local saturation temperature, whichever is higher.

5. SIMULATION RESULTS AND DISCUSSION

5.1 Condenser Heat Transfer

The experimental and calculated steam condensation rates are shown in Table 2. The total condensation rates calculated by GOTHIC at steady state are in good agreement with the specified nominal steam injection rate (0.1300 kg/s, which was used in the simulation as a boundary condition), with condensation rate being at most 0.13% greater than the steam injection rate. This small deviation is due to GOTHIC incorrectly calculating a horizontal flow of condensate away from the condenser surfaces, allowing it to pool on the floor and re-evaporate, and then re-condense. The actual steam injection rates during steady state 1 and steady state 2 were 2.1% and 4.5% below the nominal rate, respectively.

Table 2 shows 14% "parasitic" condensation, which refers to condensation that does not occur on the three condenser surfaces, but rather on the vessel walls and ceiling. The experimental condensation rates show the highest condensation rates at the top and the lowest at the middle. The GOTHIC results show the same trend at steady state 1 (end of Phase A), but not at steady state 2 (end of Phase B). Steady state 1 GOTHIC condensation rates for the top and bottom condensers are within the uncertainty of the experimental results. GOTHIC over-predicts the condensation rate for the middle condenser by 8%. At steady state 2, GOTHIC is within 12%, 28% and 21% of the measured condensation rate for the top, middle and bottom condenser, respectively. In the transition from steady state 1 to 2, the experiment showed a drop in condensation rates for the two lower condensers (bottom and middle condensers) and an increase in condensation rate for the top condenser. GOTHIC qualitatively predicted this trend, but results in an even stronger top-to-bottom stratification.

5.2 Pressure

The absolute pressure transients for Phase B are plotted in Figure 4. The times have been adjusted so that helium injection starts at 0 seconds. The experiment was specified with an injection rate of 10.6 g/s for 1740 seconds (as used in the GOTHIC model), but the experimental results show the pressure continuing to rise after 1740 seconds, indicating a longer helium injection phase. In the experiment, helium was injected at a lower rate over a longer period, but the difference in the total helium injected was less than 0.1 kg (a pressure difference of less than 1 kPa). The transient plots show the following differences between GOTHIC and the experiment:

- The GOTHIC rate of pressure increase during the helium injection period is lower than the experiment, which is explained by the lower, but longer, than specified injection in the tests.
- The observed pressure peaking about 3000 seconds after the end of helium injection is not reproduced by GOTHIC.
- GOTHIC calculates an increase in pressure between the two steady state periods that is 16.4% lower than measured in the experiment.

The delayed peak pressure (about 3000 seconds after end of helium injection) observed in the experiment was not explained by the experimenters and was not calculated by GOTHIC, a similar discrepancy is evident in the temperatures (Section 5.3). A possible explanation is the effect of the helium. The experimental measurement showed a reduction in the total condensation rate during and after the helium injection, *i.e.* the total condensation rate is below the injection rate by about 14%. This degradation in the condensation rate results in a faster pressurization rate during the helium injection and also causes the "overshoot" in pressure after the end of the helium injection (peak pressure occurs 5000 s after start of helium injection). At steady state 2, the total condensation rate is again equal to the steam injection rate. The effect of helium on the GOTHIC model is to significantly increase the convection heat transfer coefficient (e.g. convection heat transfer coefficient, for the top condenser, increased from 27 W/m^2K to 39.5 W/m^2K) and to redistribute the condensation rates for the three condensers as shown in Figure 5 (increase for top condenser and decrease for middle and bottom). However the total condensation rate remains essentially constant and equal to the steam injection rate. Therefore, GOTHIC did not reproduce the observed degradation of heat removal from the MISTRA vessel during and shortly after the helium injection.

The steady state 2 pressures show that GOTHIC under-predicted the pressure by about 5%. This corresponds to the over-prediction of the total condensation rate (for steady state 2) by 5%.

5.3 Temperature

The transient temperatures at 2 locations are shown in Figure 6. The transient plot has been normalized so that helium injection occurs at 0 seconds. The transient during helium injection does not appear to be modelled correctly by GOTHIC because the starting temperature conditions (steady state 1) were not the same as the experiment. The GOTHIC results reach steady state shortly after the end of the helium injection. In the experiment, temperatures continue to rise or fall, reaching an inflection point at about 6000 seconds, almost coinciding with the maximum pressure. The experiment did not reach steady state conditions until about 16,000 seconds.

Furthermore, GOTHIC predicts a much smaller net temperature increase, in general, than observed in the experiments. This is a result of the higher calculated convection heat transfer rates in the presence of helium.

Steady state 2 vertical temperature profiles at R0 (r = 0.0 m), R2 (r = 0.95 m) and R4 (r = 1.814 m) are shown in Figure 7 and a radial temperature profile at mid level (N7 at z = 4.625 m) is shown in Figure 8 (Sharp drop in the GOTHIC temperature at r = 1.9 m is due to the condenser). The experimental results from three tests are plotted with error bars showing $\pm 2\sigma$ (two standard deviations). The steam is injected upwards, with the nozzle outlet located along the centreline at a height z = 1.285 m. The point at a height of 0.6 m along R0 (centreline) should not be used for comparison as the experiment is measuring the conditions within the steam line and the GOTHIC result is for a location inside the vessel below the nozzle and is influenced by cool vapour flowing upward from the floor. GOTHIC under-predicts the drop in temperature immediately above the injection point (1.3 m < z < 4 m), over-predicting the temperature by up to 7°C. Above a height of 4 m, GOTHIC is within the measurement uncertainty. At the midpoint (R2), the experiment shows the temperature rising from about 125°C to 130°C over the height of the vessel, with the middle section being fairly uniform at 128°C. GOTHIC matches the temperature range across R2, but the temperature rise occurs in the upper half of the vessel. The maximum difference is about 2°C. Both the experiment and GOTHIC show a similar trend near the wall (R4). GOTHIC results are within the measurement uncertainty above 3 m. Below 3 m, GOTHIC temperatures are about 1°C lower than the experiment. The radial temperature profile at N7 (mid-height, Figure 8) shows that GOTHIC is within the measurement uncertainty. Overall, the steady state results show that GOTHIC is in good agreement with the experiment. The largest difference occurs above the steam injection nozzle resulting in a maximum difference of 8%, based on the maximum possible temperature range in the experiment ($\Delta T_{\max} = T_{injection} - T_{wall}$).

5.4 Steam Concentrations

Steady state 2 vertical steam concentration profiles along R0 (r = 0.0 m), R2 (r = 0.95 m) and R4 (r = 1.814 m) are plotted in Figure 9. Along the centreline (R0), which is the steam injection axis, GOTHIC over-predicts the steam concentrations by a maximum of 20% (volume fraction) a short distance above the injection. GOTHIC steam concentrations at the midpoint (R2) are in fairly good agreement between heights of 2 and 6 m. GOTHIC does not agree with the experiment near the top (z = 7.2 m). The steam concentration measurement at R2 at the 7-m level is suspect, because the measured concentrations on either side (R0 and R4) are more than 5% (volume fraction) higher. Below a height of 2 m, the experiment shows a steam concentration drop from 43% to 37%. This can be caused by vapour flowing past the condenser (no measured steam concentration leaving the condenser) and across the floor. GOTHIC does show the vapour flowing down past the condensers and across the floor, but the vapour leaves the end of the condenser with 38% steam, mixes with the surrounding vapour to create a mixture with about 42% steam. Thus, GOTHIC predicts a fairly uniform steam concentration for the first 3 m above the floor. GOTHIC steam concentrations are in good agreement with the measured data near the wall (R4).

5.5 Helium Concentrations

Vertical helium concentration profiles are plotted in Figure 10. Along the centreline (inside the steam plume), GOTHIC matches the trends found in the experiment, but under-predicts the helium concentration by a maximum of 12% (volume fraction). This is self-consistent with the overprediction of the steam concentration, discussed above. In the rest of the volume, the experiment shows fairly well mixed conditions with helium concentrations ranging from 32% to 35% (volume fraction). The GOTHIC results are even more uniform with an average helium concentration of 30% (volume fraction) and for the most part are within the measurement uncertainty.

5.6 Velocities

Vapour velocity measurements with Laser Doppler Velocimetry (LDV) was not successful because of the large amount of mist inside the MISTRA facility. Thus, no experimental velocity data are available for comparison.

6. CONCLUSIONS

The steady state GOTHIC results are in good agreement with Phase B of the MISTRA experiment. The exception is above the injection point where GOTHIC was not able to capture the conditions within the plume. Possible reason is that the mesh was not sufficiently fine to capture the details of the air/helium entrainment process into the steam plume.

No grid convergence study was performed for either the TOSQAN or MISTRA models. The grid that was selected for the TOSQAN model was based on engineering judgement and confirmed by its good match with the experiment. This nodalization was then scaled up to fit the larger MISTRA facility with good results, but not quite as good as for TOSQAN. The ISP organisers envisaged this as proof that a code can "scale up". However, it may just indicates that the grid used in GOTHIC to model the TOSQAN facility was much finer than required and that its scale up (expansion) still gave a sufficiently fine grid that was appropriate to model the MISTRA facility.

7. REFERENCES

1. George, T.L., L.E. Wiles, S.W. Claybrook, C.L. Wheeler and J.D. McElroy, "GOTHIC Containment Analysis Package, User Manual, Version 6.1", EPRI RP4444-1, NAI-8907-02 Rev 10, 1999 July
2. George, T.L., L.E. Wiles, S.W. Claybrook, C.L. Wheeler and J.D. McElroy, "GOTHIC Containment Analysis Package, Technical Manual, Version 6.1", EPRI RP4444-1, NAI-8907-06 Rev 9, 1999 July.

3. George, T.L., L.E. Wiles, S.W. Claybrook, C.L. Wheeler and J.D. McElroy, "GOTHIC Containment Analysis Package, Qualification Report, Version 6.1", EPRI RP4444-1, NAI-8907-09 Rev 5, 1999 July.

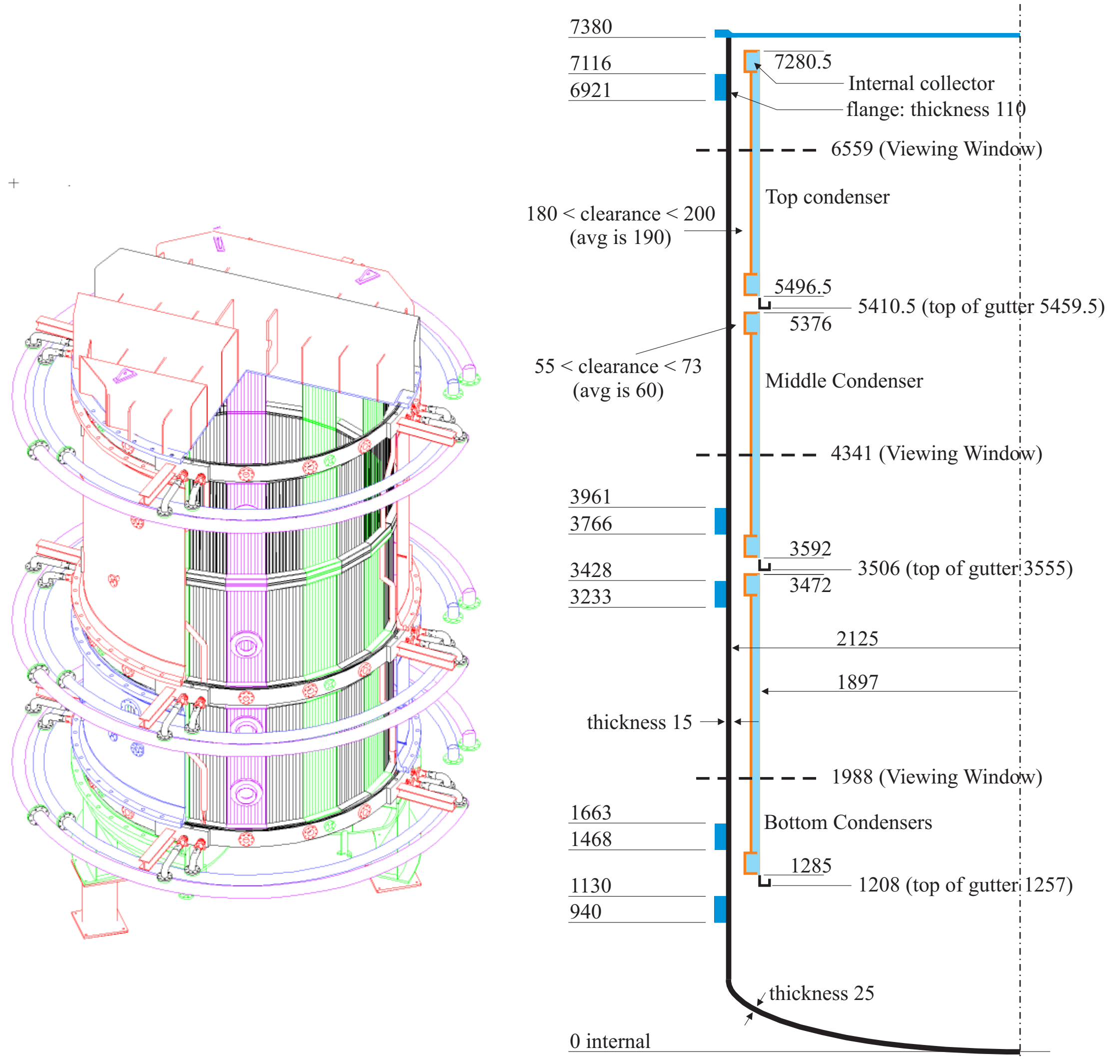
Table 1: Steam and Helium Injection Conditions

Phase	Time (s)	Injection Temperature* (°C)	Steam flow rate (kg/s)	Helium flow rate (kg/s)
A	Heating and cooling of containment			
	0 to 26,000	199	0.13	0
B	26,000 to 26,600	130		0.0106322 (18.5 kg of he injected over 1740 seconds)
	26,600 to 26,720	130–180		
	26,720 to 27,740	180–190		
	27,740 to 60,000	201		0

*Temperature range defines a linear increase with time. The specified temperature jumps between time ranges are modelled in GOTHIC by a linear rise/fall over a 1 second duration.

Table 2: MISTRA Condensation Rates

Location	Condensation Rates (kg/s)			
	Steady State 1 (end of Phase A)		Steady State 2 (end of Phase B)	
	Exp	GOTHIC	Exp	GOTHIC
Top	0.0408 ±0.0008	0.04050	0.0504 ±0.0025	0.05629
Middle	0.0316 ±0.0008	0.03493	0.0234 ±0.0029	0.02992
Bottom	0.0375 ±0.0009	0.03690	0.0321 ±0.0005	0.02535
Parasitic	0.0174 ±0.0003	0.01782	0.0182 ±0.0013	0.01860
Total	0.1273 ±0.0028	0.1301	0.1241 ±0.0072	0.1302



MISTRA Sectional Elevation (Units in mm)

Figure 1: MISTRA Cut-out View and Elevation Cross-Section (dimensions are in mm)

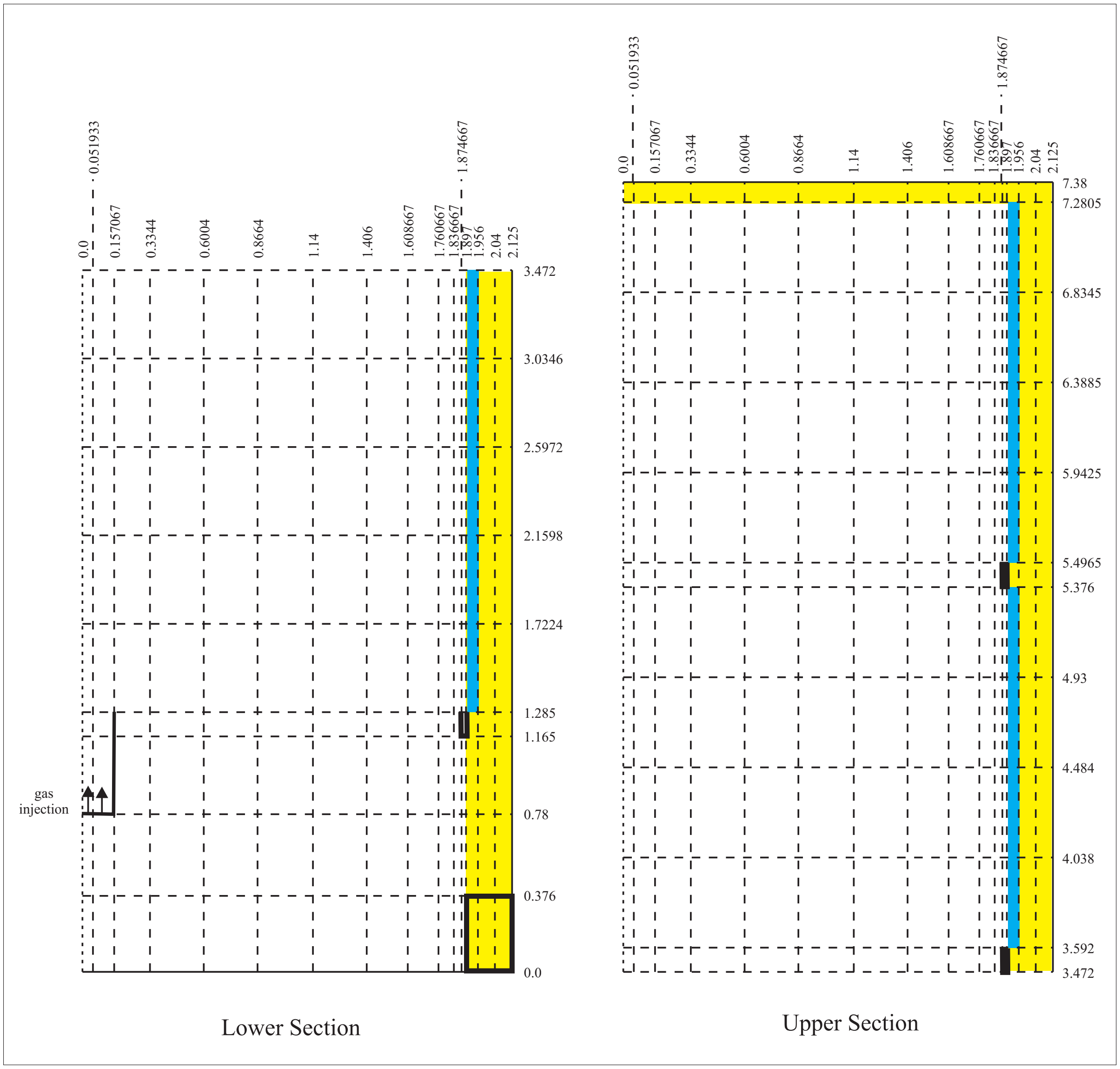


Figure 2: GOTHIC Model Nodalization of the MISTRA Facility (dimensions in m)

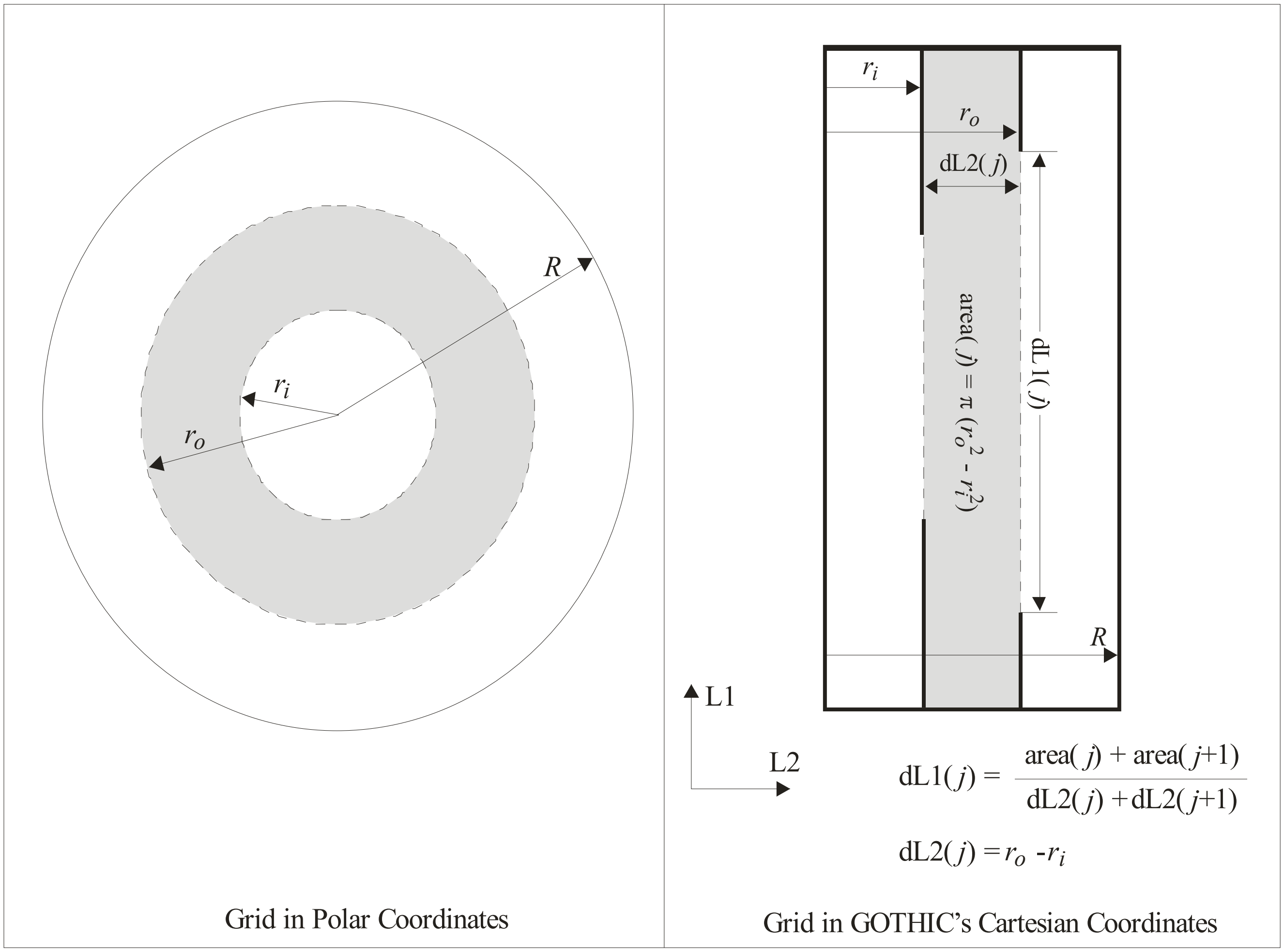


Figure 3: Approximation of Polar Coordinates Using GOTHIC's Cartesian Coordinates

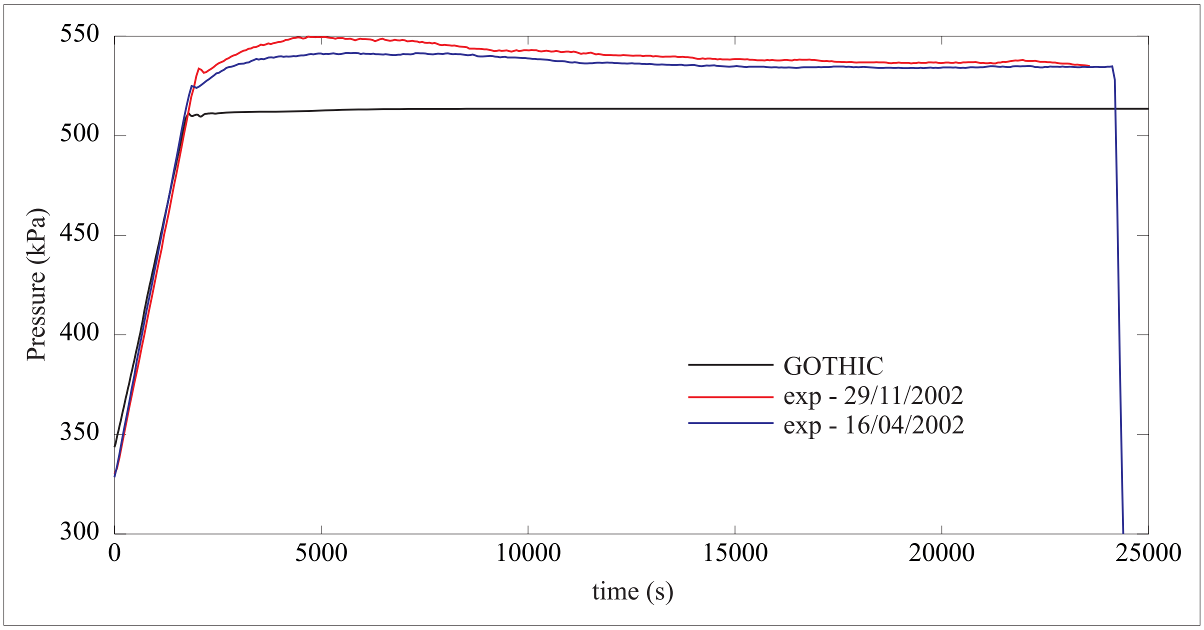


Figure 4: Pressure (Absolute) Transient After Start of Helium Injection

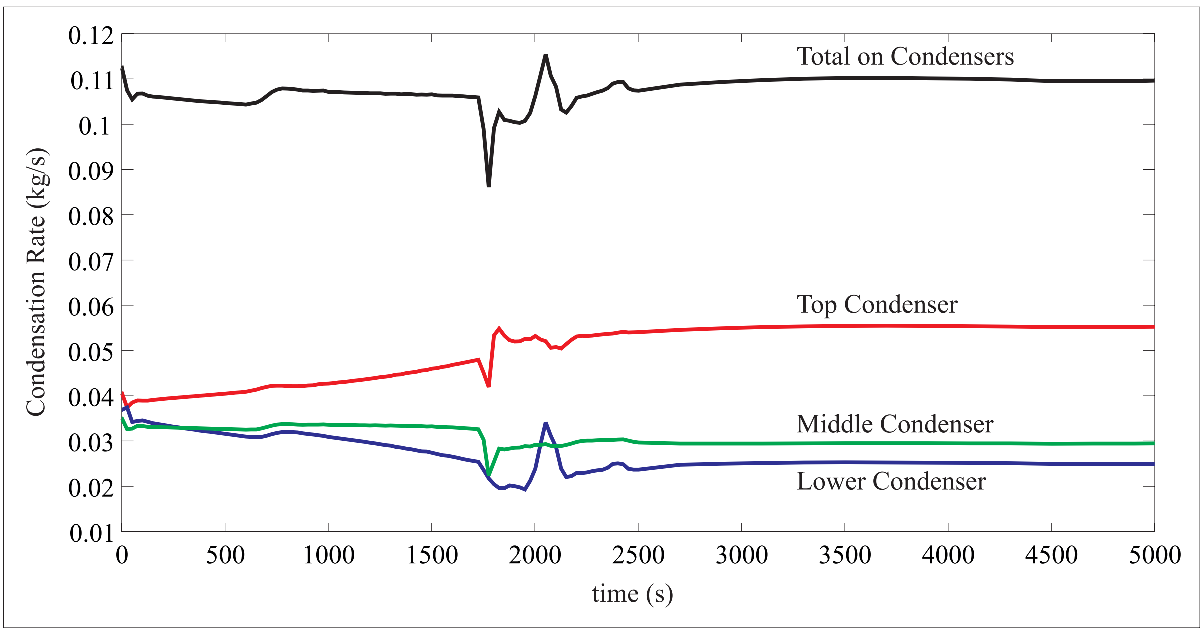


Figure 5: Condensation Rates Predicted by GOTHIC After Start of Helium Injection

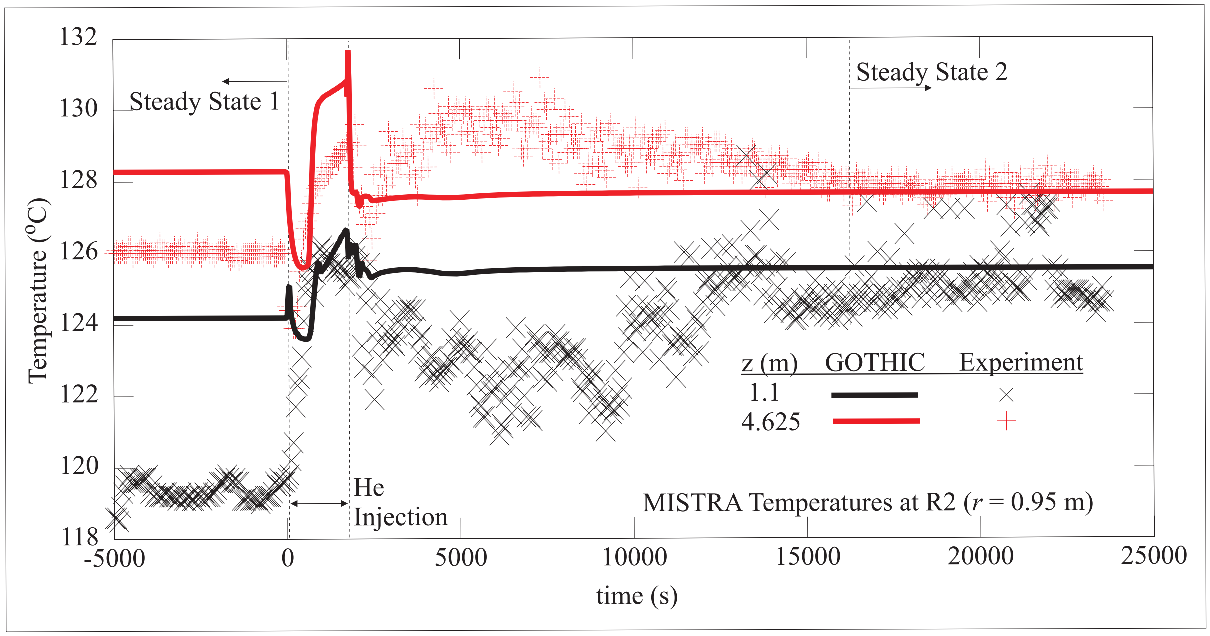


Figure 6: Transient Temperature at r = 0.95 m and z = 1.1 and 4.625 m

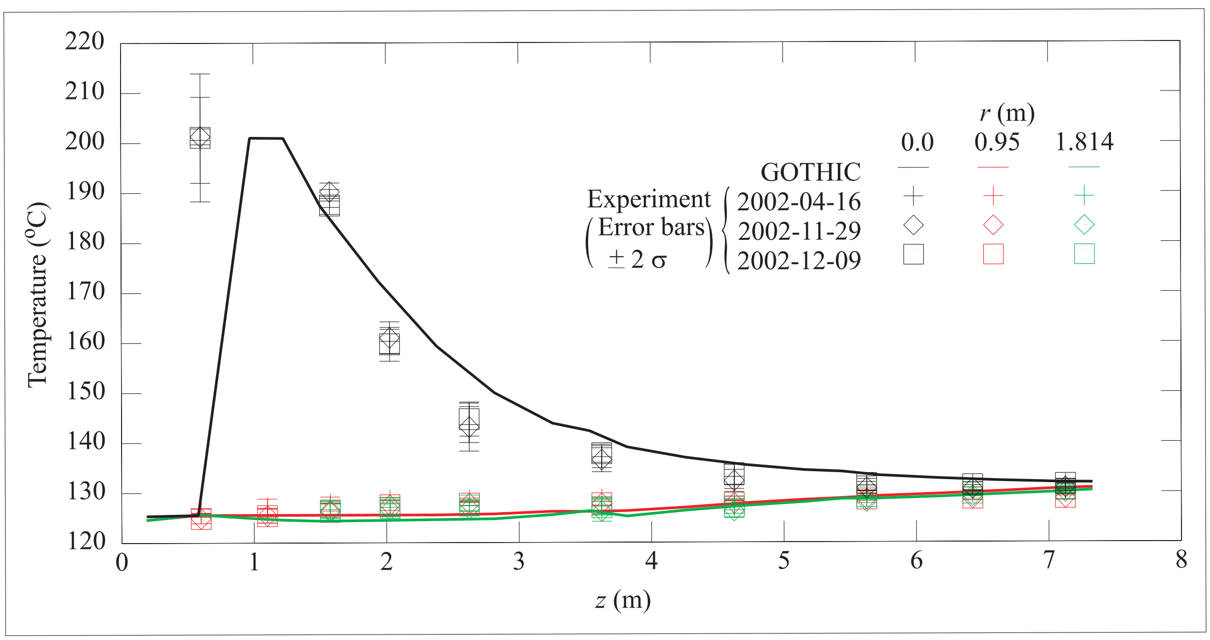


Figure 7: Steady State 2 Vertical Temperatures Profiles (along r = 0.0, 0.95 and 1.814 m)

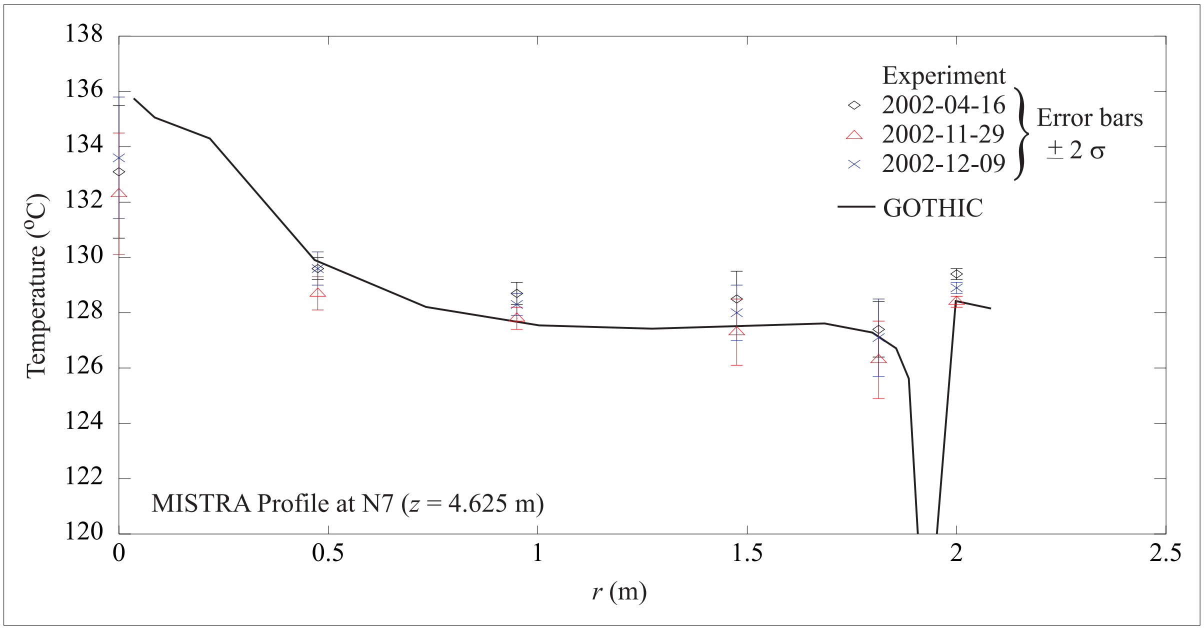


Figure 8: Steady State 2 Radial Temperatures Profiles at Mid Level (z = 4.625 m)

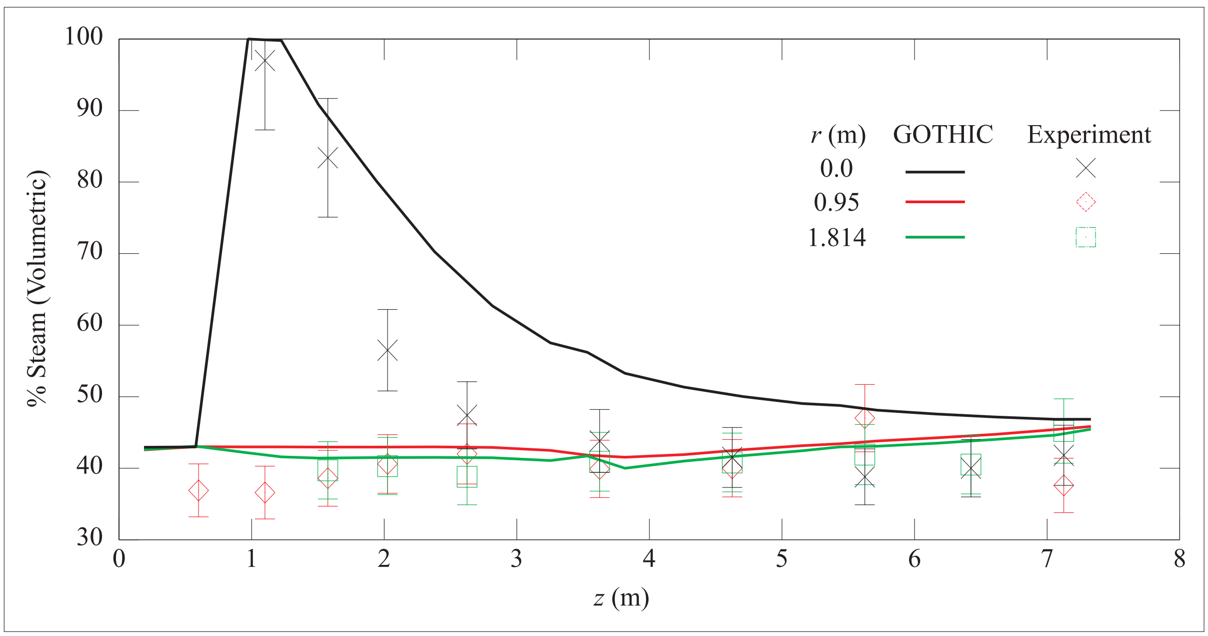


Figure 9: Steady State 2 Vertical Steam Concentration Profiles (along r = 0.0, 0.95 and 1.814 m)

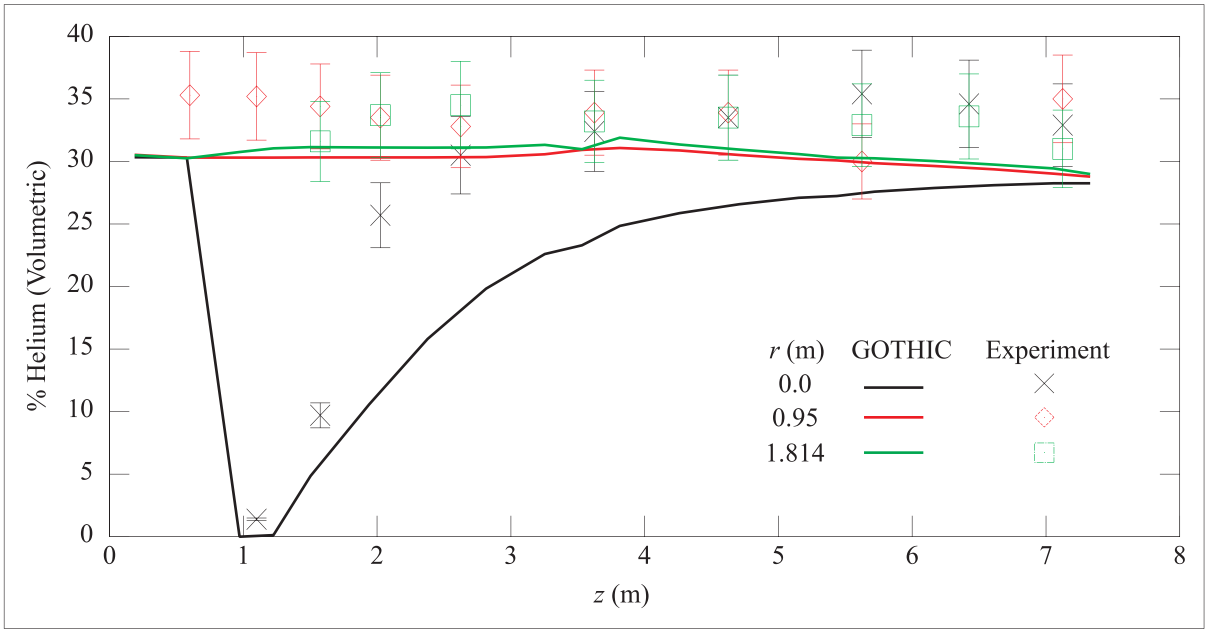


Figure 10: Steady State 2 Vertical Helium Concentration Profiles (along r = 0.0, 0.95 and 1.814 m)