1. INTRODUCTION

International Standard Problem (ISP) exercises are comparative exercises, in which predictions of different computer codes for a given physical problem are compared with each other, or with the results of a carefully controlled experimental study. The main goal of ISP exercises is to increase confidence in the validity and accuracy of the tools that are used to assess the safety of nuclear installations. Moreover, the exercises enable code users to gain experience and demonstrate their competence.

The ISP 41 exercise, a comparison of iodine behavior models, was first proposed at the Fourth Iodine Chemistry Workshop held at the Paul Scherrer Institute (PSI), Switzerland in 1996 June. The results of a Radioiodine Test Facility (RTF) experiment were made available by CANDU® Owners Group (COG) for the exercise. An RTF experiment performed under controlled and limited conditions was chosen as a starting point for the evaluation of the various iodine behavior codes, in the hope that the basic components of each code could be compared. The experiment was ideal for demonstrating the ability of all of the codes to model the influence of pH on iodine volatility, one of the most important aspects of iodine behaviour. Participants were given details of the experimental set-up, conditions and procedures of the RTF test, and they were asked to calculate experimentally observed parameters, such as the total concentration and speciation of iodine in the gas and aqueous phases, and the distribution of iodine at the end of the test between the gas phase, the aqueous phase and surfaces that were exposed to each of these phases.

Results from the first step of ISP 41 are detailed elsewhere [1]. The objective of the exercise, which was to evaluate the basic components of each code, and to demonstrate their ability to simulate experimental results under controlled conditions, was achieved. The exercise established that the pH dependence of iodine volatility can be accurately reproduced by all codes used in the study.

The following additional conclusions arose from the first step of ISP 41:

1. The performance of the iodine behavior codes is extremely reliant upon the judicious choice of user-defined kinetic parameters, many of which have been chosen to provide a best fit of the code output to experimental data obtained under a narrow range of conditions (such as temperature, dose rate, iodide concentrations, etc.).

2. In order to use code calculations as predictive or interpretive tools, it must be demonstrated that the kinetic parameters used in the codes are applicable to the entire range of conditions anticipated in post-accident containment.

These conclusions, and the recognition that the first step of the comparison exercise did not evaluate several aspects of code performance (e.g., the ability to predict pH, and organic iodide formation) led to the recommendation that two follow-up exercises be performed as part of ISP

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41. The first phase of these follow-up exercises, consisting of a set of parametric studies, is described in this document.

The parametric studies described in this document were designed to evaluate the sensitivity of iodine behaviour codes to boundary conditions such as pH, dose rate, temperature and initial I^-concentration. The comparison of code results over a wide range of conditions is necessary to understand where the codes agree and where they diverge, so that a strategy for further code development, application and validation can be developed. The results of the parametric study will also determine the readiness of each code for the proposed second phase of the exercise, i.e., a blind code comparison test using two intermediate scale studies that are more complex than the RTF experiment used for the initial step of ISP 41.

The range of conditions for the parametric calculations are

pH	4 - 10
temperature	60 - 130 °C
dose rate	0.1 - 10 $kGy{\cdot}h^{-1}$
initial I^- concentration	10^{-6} - 10^{-4} $moles{\cdot}dm^{-3}$

The effect of steam condensation, the presence of Ag, and the availability of organic materials in the aqueous phase were also examined in the exercise. A full description of the parametric matrix can be found in Appendix A.