CRITERIA FOR TRANSITION FROM DEFLAGRATION TO DETONATION IN H_2-AIR-STEAM MIXTURES

C.K. Chan, W.A. Dewit and G.W. Koroll
AECL
Whiteshell Laboratories
Pinawa, Manitoba R0E 1L0
CANADA

ABSTRACT. Flame acceleration and transition to detonation were examined for various H_2-air-steam mixtures in a 28 cm diameter, 6.4 m-long, combustion duct filled with obstacles. The run-up distances for DDT (distance between ignition and onset of detonation) were measured for these mixtures and found to be inversely proportional to the laminar burning velocities of the corresponding mixtures. Based on these results, experimental DDT limits were established. Instead of relying on the detonability limits as the conservative criteria for DDT, the experimental DDT limits offer a set of less restrictive criteria. Results also showed that DDT did not occur if a flame had not accelerated to a speed corresponding to a flame Mach number greater than 1.5. This critical value indicates that for H_2-air-steam mixtures, the mechanism for DDT is closely related to the strength of its leading shock. Comparison with other experiments confirms that initiation of detonation by shock focusing caused by the reflection of the leading shock off obstacles is the dominant mechanism for DDT in these insensitive mixtures.

INTRODUCTION

During postulated loss-of-cooling accidents in nuclear power reactors, hydrogen can be produced as a result of metal-steam reactions. This hydrogen can leak into the containment building to form a combustible mixture. If ignited, the pressure loading on local structures resulting from a hydrogen burn, depends on whether the burn is a deflagration or a detonation. Direct initiation of detonation is very unlikely because it requires a high energy source such as solid explosive that is not present inside a reactor. However, a detonation is still possible by way of a Deflagration to Detonation Transition (DDT). At the present time, the necessary conditions (or criteria) for a DDT to occur under a given situation have not been fully quantified. Computer codes that fully describe the DDT phenomenon have not been developed. It is not possible to predict a priori whether a transition can occur in a given situation. Qualitative methods based on empirical criteria are the only available methodology to assess the likelihood of a DDT. In recent years, many studies had been devoted to determine these criteria [1-6]. For H_2-air-steam mixtures, the most probable cause for transition to detonation is believed to be related to the intrinsic instability of

acceleration of a freely expanding flame. Due to a feedback mechanism between the combustion induced flow and the reaction zone itself, a flame can accelerate very rapidly if obstructions are placed along its path. If appropriate conditions (in terms of the composition of the mixture, the flame speed, the local turbulent flow structure and the configuration of the obstruction) are present, a DDT can occur.

As recently as in 1979, it was generally accepted that the detonability limits for H_2-air mixtures were 18% and 59% of hydrogen by volume at lean and rich limits respectively [7]. The detonability range for H_2-air mixtures has been widened gradually in recent years as more data have become available. It was reported recently [8] that the detonable range for dry H_2-air mixtures at 1 atm initial pressure and 20°C is between 11.6 and 74.9 percent by volume. At 100°C initial temperature and 1 atm pressure, the range of detonable concentration expands to between 9.4% and 76.9%. This report also pointed out that steam plays an important role in reducing the detonable range. The addition of steam not only reduces the volume percent of H_2 and air, it also acts as an effective heat removal medium. Detonation was not observed even in a stoichiometric H_2-air-steam mixture when steam concentration was above 38.8%. Since the experimentally determined detonability limit is the most readily available information on the limits, it is often used as the first criterion for DDT.

Another criterion for DDTthat may be useful for practical application is the flame speed (extent of flame acceleration) required before transition to detonation becomes likely. In a region filled with obstacles, a flame may accelerate due to obstacles-induced turbulent in the unburned gas flow. However, if the available length of travel for the flame is insufficient for the flame to accelerate to high enough speeds, such that shock waves produced are not capable of causing local explosions, then a transition is unlikely. Thus transition distance (or run-up distance) may be used as a criterion for assessing the likelihood of DDT [9-11]. Although run-up distance is not an intrinsic property that characterize DDT and it depends on the mixture composition as well as the geometry (obstacle shape, size and spacing, wall roughness that can promote turbulence) of the enclosure, data from the same apparatus can provide a relative measure of the susceptibility to flame acceleration and DDT for various mixtures.

Recent studies [5,12] indicate the existence of a criterion for DDT that is more quantitative and less conservative than the detonability limits. This criterion is based on measurable experimental parameters. If transition arises through flame acceleration, then the possibility of a transition can be quantified as the critical strength of the shock wave ahead of the accelerated flame that leads to the local explosion in the mixture of interest. This criterion translates to a critical flame speed.

The critical flame speed and the detonability limit are merely necessary conditions for DDT. Any one alone does not represent a sufficient condition for a DDT to occur under a given set of initial and boundary conditions. For a DDT to occur, both of the criteria have to be satisfied. Nevertheless, these criteria for H_2-air-steam mixtures have not been systematically determined. This paper presents results of studies on DDT resulting from flame acceleration and, based on these results, establishes the criteria for DDT for these insensitive mixtures.

EXPERIMENTAL APPARATUS

Experiments on transition from deflagration to detonation for H_2-air-steam mixtures (at 100°C initial temperature and 100 kPa initial pressure) were performed in a 28 cm diameter, 6.4 m-long, combustion duct. A flame was created by igniting the gas mixture with a weak electrical spark (~1 mJ).

Rectangular baffle-type obstacles with a blockage ratio (blocked area to total cross-sectional area) of 0.31 were installed along the duct to induce turbulence in the unburned gas. Schematics of the experimental apparatus and the obstacle configuration are shown in Fig. 1. Piezoelectric pressure transducers were mounted along the side wall and at the end plate of the duct to monitor the location of DDT as well as the flame speed just prior to the onset of detonation. The last pressure transducer is mounted on the end plate and usually recorded much higher pressures (reflected shock) than the rest of the transducers, as the end plate is facing the incoming shock (or flame). The pressure at the end plate, in general, represents the highest mechanical loading resulting from an explosion.

RESULTS AND DISCUSSION

Upon ignition, it was observed that a flame accelerated very rapidly in the duct. Even though pressure transducers cannot detect the arrival of a slow flame front, they can detect the leading shock front associated with an accelerated flame (with flame speeds greater than 300 m/s). For supersonic deflagration, the leading shock and the reaction zone propagate at roughly the same speed [13]. After a flame had accelerated beyond a certain critical speed, a sudden jump in the flame speed to detonation velocity was observed. Assuming the final velocity of the detonation corresponds to the

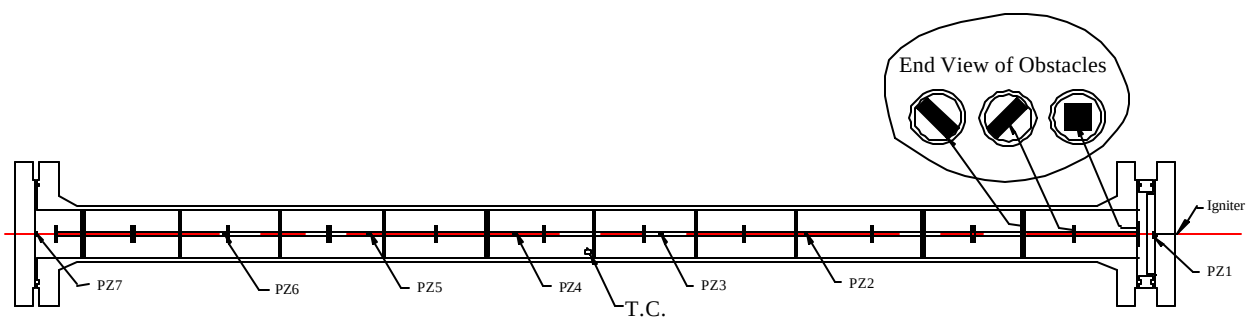

Figure 1. Schematics of the Experimental Apparatus and the Obstacle Configuration

Chapman Jouguet detonation condition of the mixture, the location of DDT (onset of detonation) can be estimated to an accuracy equivalent to half the distance between consecutive pressure transducers (~0.5 m). Figure 2 shows the run-up distances for various H_2-air-steam mixtures. The run-up distance (also commonly referred to as transition distances or induction distances) is defined as the distance between the ignition point and the location of onset of detonation. As mentioned earlier, this run-up distance is not an intrinsic property of the mixture; it depends on the size of the duct as well as the obstacle configuration. Since all experiments were performed under the same boundary conditions, the run-up distance provides a comparison of the sensitivity of the mixture in terms of flame acceleration and DDT. For example, for lean mixtures (< 30% H_2 in H_2-air), the run-up distances increase by a factor or two for every 5 vol % decrease in H_2 concentration. Similarly, a

10 vol % increase in steam will have the same effect on the run-up distance as a 5 vol % decrease in H_2 concentration. For dry, 10%, and 20% steam mixtures, data show the trend of a U shaped curve. These results suggest that the run-up distance is inversely proportional to the laminar burning velocity of the corresponding mixture. In this series of experiments, no DDT was observed for mixtures of 30% or more steam by volume.

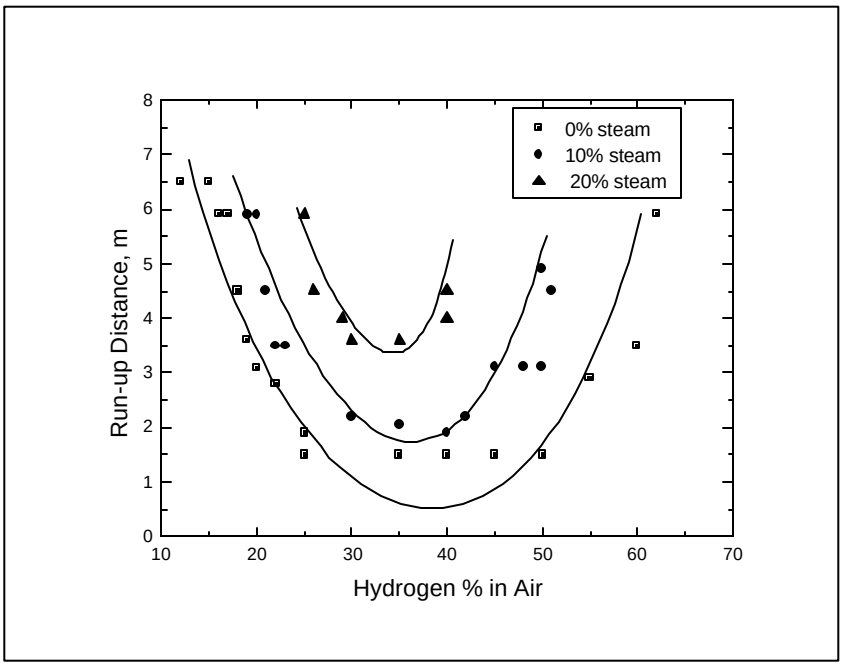

Figure 2. The Run-up Distances for Various H_2-air-steam Mixtures in a 28 cm dia. Duct Filled with Obstacles (B.R. = 0.31)

For dry H_2-air mixtures, the run-up distances as defined above were not observed for mixtures containing less than 15% or more than 62% of hydrogen by volume. The run-up distances for 15% and 62% H_2 mixtures were estimated to be about 5.8 m which is the mid-point between the last two pressure transducers. For 12% and 14% H_2 mixtures, while their flame speeds between the last two transducers were below 800 m/s, the pressures recorded by the last pressure transducer were above the corresponding detonation pressures of the mixtures. This implies that transition to detonation was triggered by the reflected flame or shock off the end flange. In these cases, DDT did not occur in the mixture at their initial pressure of 100 kPa. Depending on the flame speed, the reflection of the leading shock can compress the mixture to 3-5 times its initial pressure [13]. As a result, the critical conditions of DDT for these mixtures are different from those of the rest of the mixtures. Nevertheless, DDT was observed in these experiments. The run-up distances for these experiments were assumed to be at least at the end flange.

Figure 2 shows that the limiting mixtures for DDT in this series of experiments are 15% and 62% H_2 by volume for dry mixtures, 19% and 52% H_2 in H_2-air for mixtures containing 10% steam, and 24% and 40% H_2 in H_2-air for mixtures containing 20% steam. In terms of the concentration by volume in the mixtures, the last two sets of numbers become (17.1% and 46.8%) and (19.2% and 32.0%). These limiting mixtures can be considered as the experimental DDT limits. For comparison, these experimental DDT limits (open symbols) are shown in Fig. 3 together with the detonability (solid symbols) and flammability limits (solid line). It should be mentioned that DDT limits determined in these experiments may be different from the limits determined using a different apparatus. DDT limits are known to be scale dependent. However, a collection of data from various DDT experiments using different apparatuses can be used to establish a boundary in terms of composition of the mixture outside which a DDT has not been observed. Instead of relying on the detonability limits as conservative criteria for DDT, these experimental DDT limits provide useful guidelines for the safety analysts to determine the likelihood of a DDT in a given situation. With the experimental DDT limits identified, a meaningful uncertainty analysis can be made; the further away a situation is from these limits, the less likely a DDT can occur in the mixture.

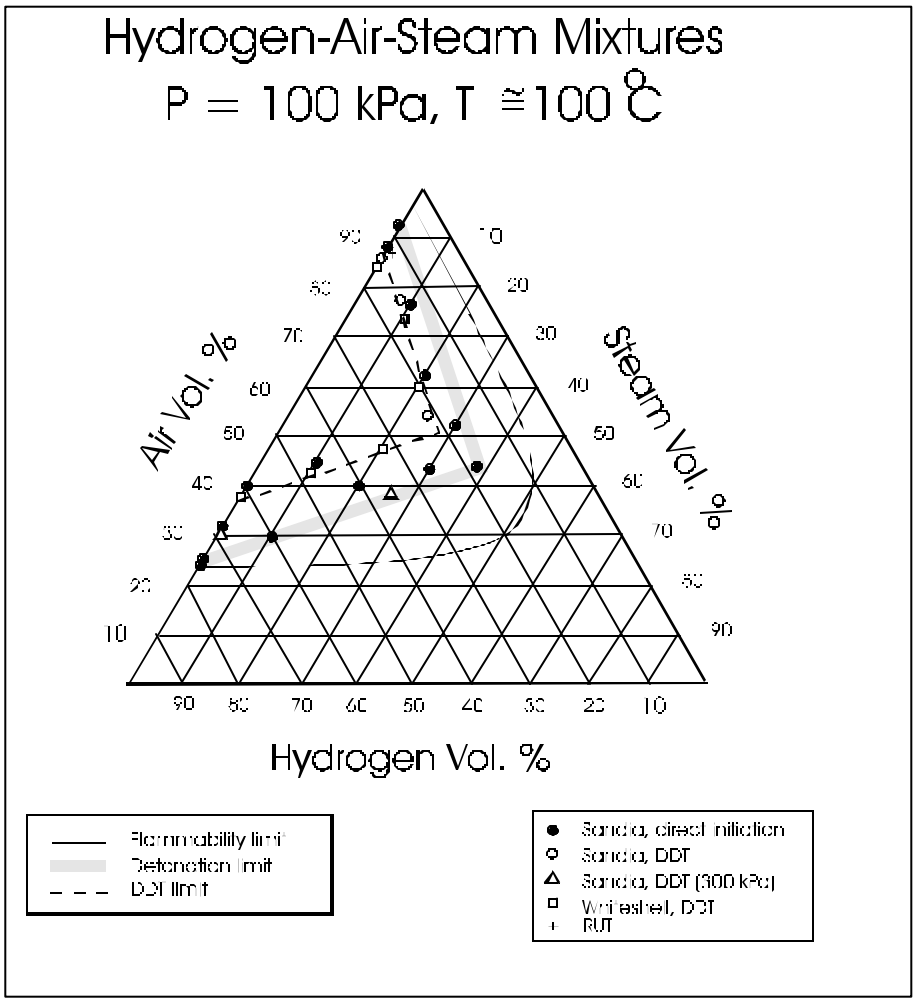

Figure 3. Experimental DDT Limits, Detonability Limits and Flammability Limits for H_2-air-steam Mixtures

The flame speeds just prior to DDT were also determined in this series of experiments. These data, expressed as the flame Mach numbers (flame speed normalized by the sonic velocity in the uncompressed mixture), are shown in Fig. 4 (solid symbols). Most of the critical flame Mach numbers are within the range of 1.5 to 2.0. In general, the higher the steam content, the higher is the critical flame Mach number. This implies that it is more difficult to trigger a DDT in mixtures containing high steam content. For those cases in which DDT was not observed, the maximum flame speeds (the average speed between the last two pressure transducers) are also shown in Fig. 4 (open symbols). As discussed earlier, these critical flame speeds just prior to DDT can be used as one of the criteria for DDT. Nevertheless, these critical speeds are only necessary conditions. For a DDT to occur, other criteria must also be satisfied. Figure 4 shows that if a mixture is within the experimental DDT limits, DDT is probable if its flame Mach number exceeds about 1.5. For mixtures outside the limits, DDT is not possible even though the flames have already accelerated to much higher flame Mach numbers.

The existence of a critical flame Mach number implies that the dominant mechanism for DDT in these relatively insensitive mixtures is related to the strength of its leading shock. It has been demonstrated [12] that compound reflection and deflection of the leading shock by collisions with obstacles along its path can cause local strengthening of the shock wave (commonly referred to as shock focusing) and create local hot spots capable of causing direct initiation of detonation. Experiments on initiation of detonation by shock focusing [14] showed that the critical shock Mach numbers for initiation of

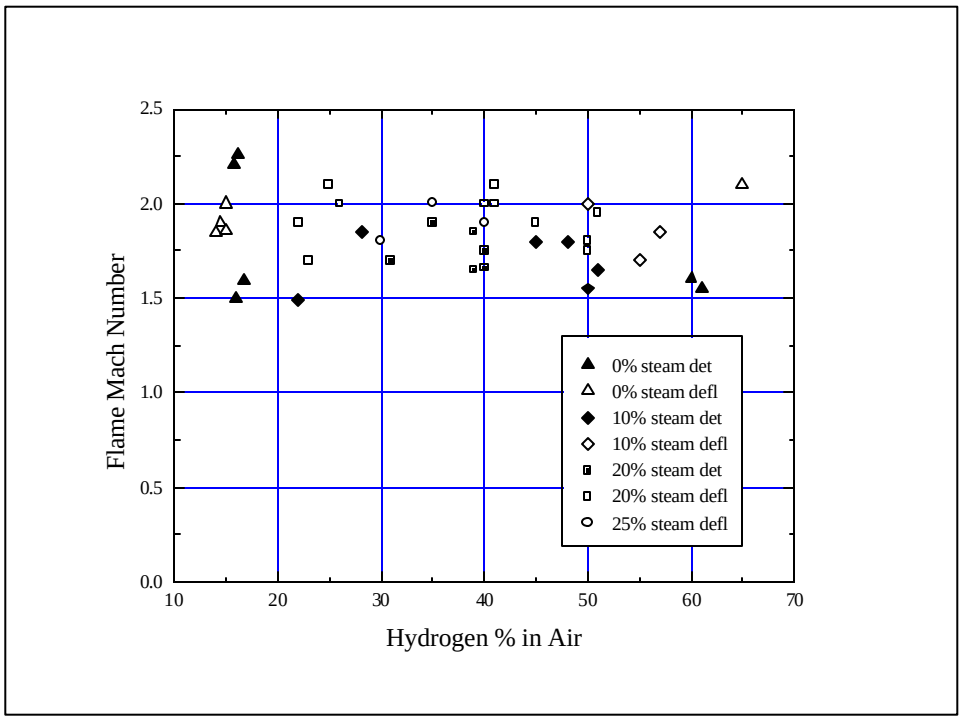

Figure 4. The Critical Flame Mach Numbers for DDT Resulting from Flame Acceleration in H_2-air-steam Mixtures

detonation have similar range of values. Even though it has been demonstrated that under certain situations, turbulence can play an important role in DDT [15], our results suggest that for H_2-air-steam mixtures, turbulence is unlikely the dominant mechanism for DDT. If turbulence is the dominant mechanism, the critical Flame Mach numbers would be below 1 because the maximum turbulent fluctuation velocity is the sonic velocity. The fact that no DDT was observed for flames with flame Mach numbers lower than 1.5, indicates that the initiation of detonation by shock focusing resulting from the reflection of the leading shock off obstacles is the dominant mechanism for DDT in accelerated flames.

SUMMARY

Flame acceleration and DDT were examined for various H_2-air-steam mixtures in a 28 cm diameter, 6.4 m-long, combustion duct. The run-up distances for DDT were measured for these mixtures. Results show that the run-up distances are inversely proportional to the laminar burning velocities of the mixtures. Experimental DDT limits were established by assuming that mixtures at the limits would have infinitely long run-up distances. Instead of relying on the detonability limits as conservative criteria for DDT, these limits can be used as less conservative criteria. Results also showed that DDT did not occur if the Mach number of the accelerated flame was less than 1.5. This critical value suggests that for H_2-air-steam mixtures near the limits of detonatibility, the focusing of the leading shock by compound reflection off obstacles is the dominant mechanism for DDT for accelerated flames. The DDT limits and the critical flame speed are necessary conditions for DDT but are not sufficient conditions. That is, both of these criteria have to be satisfied before a DDT can occur.

ACKNOWLEDGMENT

This work was funded jointly by Atomic Energy of Canada Limited, Ontario Hydro, Hydro Quebec and the New Brunswick Power Corporation under the CANDU### Owners Group agreement.

REFERENCES

1. Dorofeev, S.B., A.V. Bezmelnitsin, A.A. Efimenke, A.S. Kochurke, V.P. Sidorov, J.G. Yankin, I.D. Matsukov, "Experimental Study on the Combustion Behavior of Hydrogen-Air Mixtures with Turbulent Jet Ignition at Large Scale", USNRC report NUREG/CR 6072, 1993.
2. Carnasciali, F., J.H. Lee, R. Knystautas and F. Fineschi, "Turbulent Jet Initiation of Detonation", Comb. and Flame, pp. 170-180, 1991.
3. Lee, J.H., R. Knystautas and C.K. Chan, "Turbulent Flame Propagation in Obstacle-Filled Tube", 20th Symposium (Int.) on Combustion, The Combustion Institute, Pittsburgh, Pa., pp. 1663-1672, 1985.
4. Peraldi, O., R. Knystautas and J.H. Lee, "Criteria for Transition to Detonation in Tubes", 21st Symposium (Int.) on Combustion, The Combustion Institute, Pittsburgh, Pa., p. 1629, 1986.
5. Chan, C.K., D. Lau and D. Radford, "Transition to Detonation Resulting from Burning in a Confined Vortex", 23rd Symposium (Int.) on Combustion, The Combustion Institute, Pittsburgh, Pa., pp. 1797-1804, 1990.

6. Dorofeev, S.B., V.P. Sidorov, A.E. Dvoinishnikov and W. Breitung, "Deflagration to Detonation Transition in Large Confined Volume of Lean Hydrogen-air Mixtures", to appear in Comb. and Flame, 1995.
7. Berman, M. et al. (editors), Proceedings of the Workshop on the Impact of Hydrogen on Water Reactor Safety, Albuquerque, NUREG/CR 2017, SAND 81-0661, 1981.
8. Stamps, D.W., W.B. Benedick and S.R. Tieszen, "Hydrogen-Air-Diluent Detonation Study for Nuclear Reactor Safety Analyses", NUREG/CR-5525, SAND 89-2398, 1991.
9. Baumann, W., P.A. Urtiew and A.K. Oppenheim, "On the Influence of Tube Diameter on the Development of Gaseous Detonation", Z. Elektrochem, 65, pp. 898-902, 1961.
10. Nzeyimana, E., M. Vandermeiren and P.J. Van Tiggelen, "Influence of Chemical Composition on the Deflagration-Detonation Transition", Progress in Astronautics and Aeronautic, 106, pp. 19-36, 1986.
11. Bollinger, L.E., "Experimental Detonation Velocities and Induction Distances in Hydrogen Air Mixtures", AIAA Journal, Vol. 2, pp. 131-133, 1964.
12. Chan, C.K., "Collision of a Shock Wave with Obstacles in a Combustible Mixture", Comb. and Flame, 100, No. 1/2, p. 341, 1995.
13. Chan, C.K. and D. Greig, "The Structure of Fast Deflagrations on Quasi-detonations", 22nd Symposium (Int.) on Combustion, The Combustion Institute, Pittsburgh, Pa., pp. 1733-1739, 1988.
14. Chan, C.K., D. Lau, P. Thibault and J.D. Penrose, "Ignition and Detonation Initiation by Shock Focusing", AIP Conference Proceedings Vol. 208, Current Topics in Shock Waves, p. 161, 1990.
15. Lee, J.H. and I.O. Moen, "The Mechanism of Transition from Deflagration to Detonation in Vapor Cloud Explosion", Progress in Energy and Combustion Science, 6, pp. 359-389, 1980.

CANDU® (CANada Deuterium Uranium), registered trademark of Atomic Energy of Canada Limited (AECL).