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# **Modeling & Analysis of Liquid Deuterium-Water Reactions**

by

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# **This Presentation Will Highlight**

- o Overview of LD<sub>2</sub>-Water reactions & their connections to research reactors with cold sources**
- o Some key features and ingredients of vapor explosions in general**
- o Examination of results of 1970 experiment at Grenoble Nuclear Research Center**
- o Thermodynamic evaluations of energetics of explosive LD<sub>2</sub>-D<sub>2</sub>O reactions**

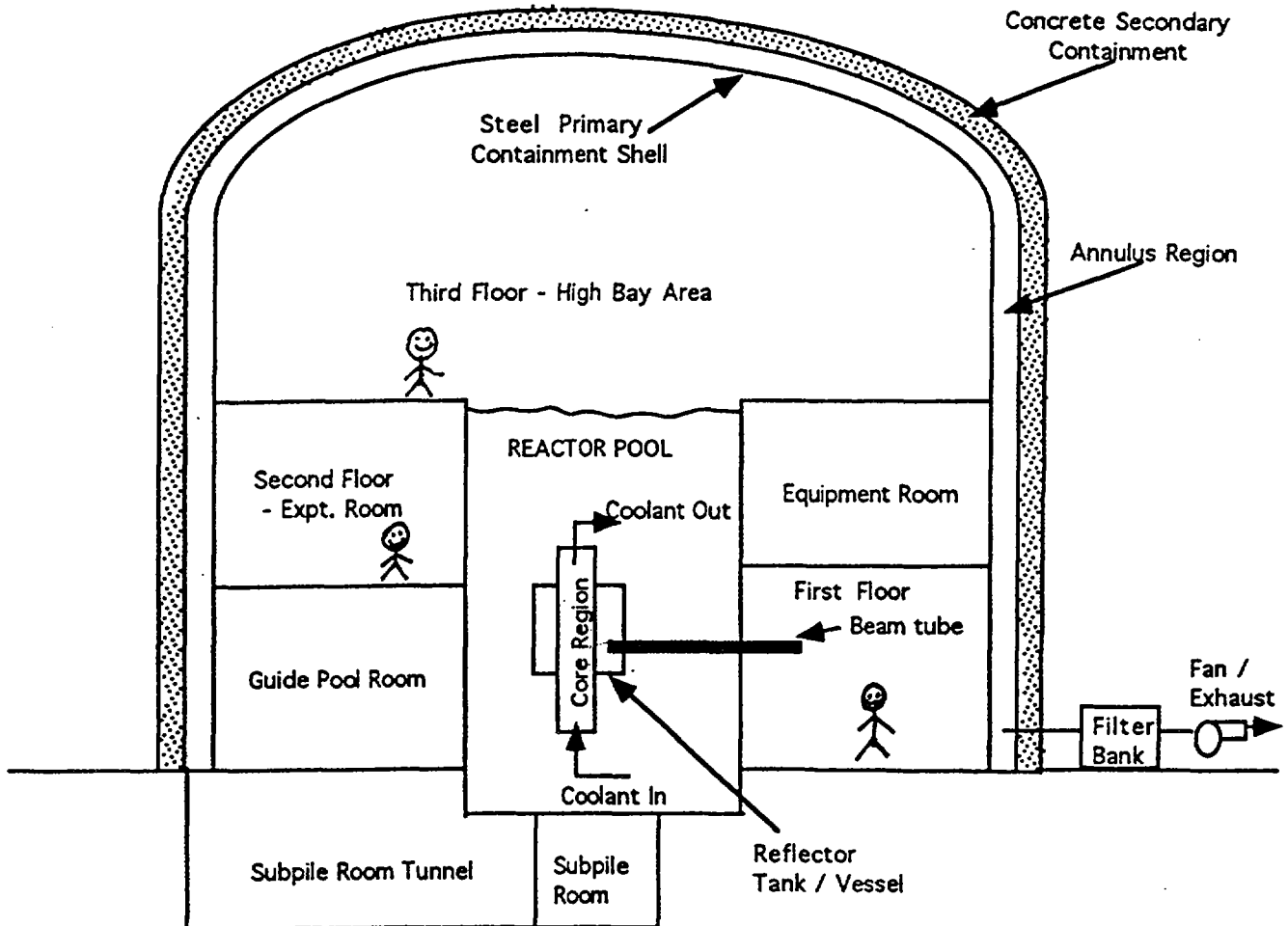
**\*\*\*\* This presentation will concentrate only upon the technical aspects of LD<sub>2</sub>/LH<sub>2</sub> Water reactions; it is not intended to draw/imply safety-related conclusions for research reactors \*\*\*\***

# Notes on Vapor Explosions

**\*\*\*\*\* It is well-known from several Freon-water, LNG-water experiments and experiences that such interactions can be explosive under the right circumstances \*\*\*\*\***

- o Vapor explosions (also referred to as FCIs) occur (if they do so) in 3 stages:**
  - Intimate premixing of hot and cold fluids**
  - Triggering to initiate film collapse and dispersion --> explosive heat transfer**
  - Propagation through mixture ---> pressure buildup and mechanical work**
- o An LD<sub>2</sub>-Water explosion would fall in the general category of FCIs where water is now the hot fluid**
- o Important effects and features to keep in mind are:**
  - Initial contact mode (e.g., injection, stratification, radial egress, etc.)**
  - Scale effects (small quantities usually need robust external triggering compared with large scale explosions)**
  - Thermodynamic states of hot and cold fluid**
  - Geometry of reaction zone (inertial constraint)**

# ANS CONTAINMENT



# Grenoble Experiments

- o Geometry was carefully engineered to represent a scaled-down representation of ILL cold source within the reflector tank
- o Experiment parameters vs ILL reactor cold source

<u>Parameter</u>	<u>Experiment</u>	<u>ILL Reactor</u>
-Cold source fluid	LH <sub>2</sub>	LD <sub>2</sub>
-Source volume (L)	.025 to 1	38
-Source geometry	double walled (glass)	double walled (aluminum)
-Distance from source to reflector tank (m)	0.4	0.7

- o Instrumentation

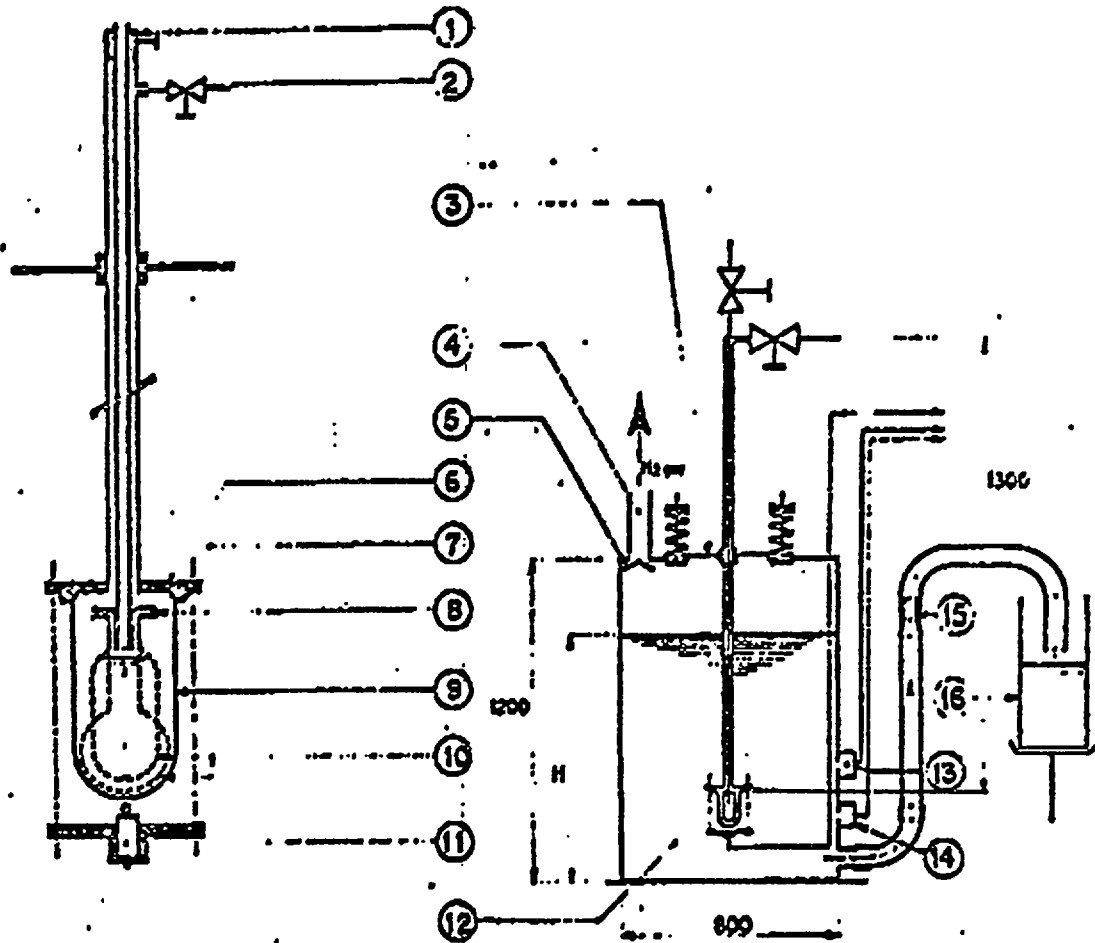
- Pressure taps at walls (response time ?), visual & camera film (<200 fps)

- o Experiment types

- 1) Impact hammer induced double-wall perforation ---> No explosion
- 2) Internal pressure buildup-induced forced ejection --> Explosive reaction

TEST CELL

OVERALL VIEW



- |                         |                             |
|-------------------------|-----------------------------|
| 1. Direct passage valve | 8. Strap and O ring         |
| 2. Vacuum plug          | 9. PYREX vacuum bell        |
| 3. Valve                | 10. PYREX container of LH2  |
| 4. Stack                | 11. Striker                 |
| 5. Deflector            | 12. Water                   |
| 6. Strap                | 13. Membrane manometer      |
| 7. Rubber gasket        | 14. Piezoelectric manometer |
|                         | 15. Venturi                 |
|                         | 16. Container               |

Figure 1. Schematic of Experimental Facility (dimensions in mm)

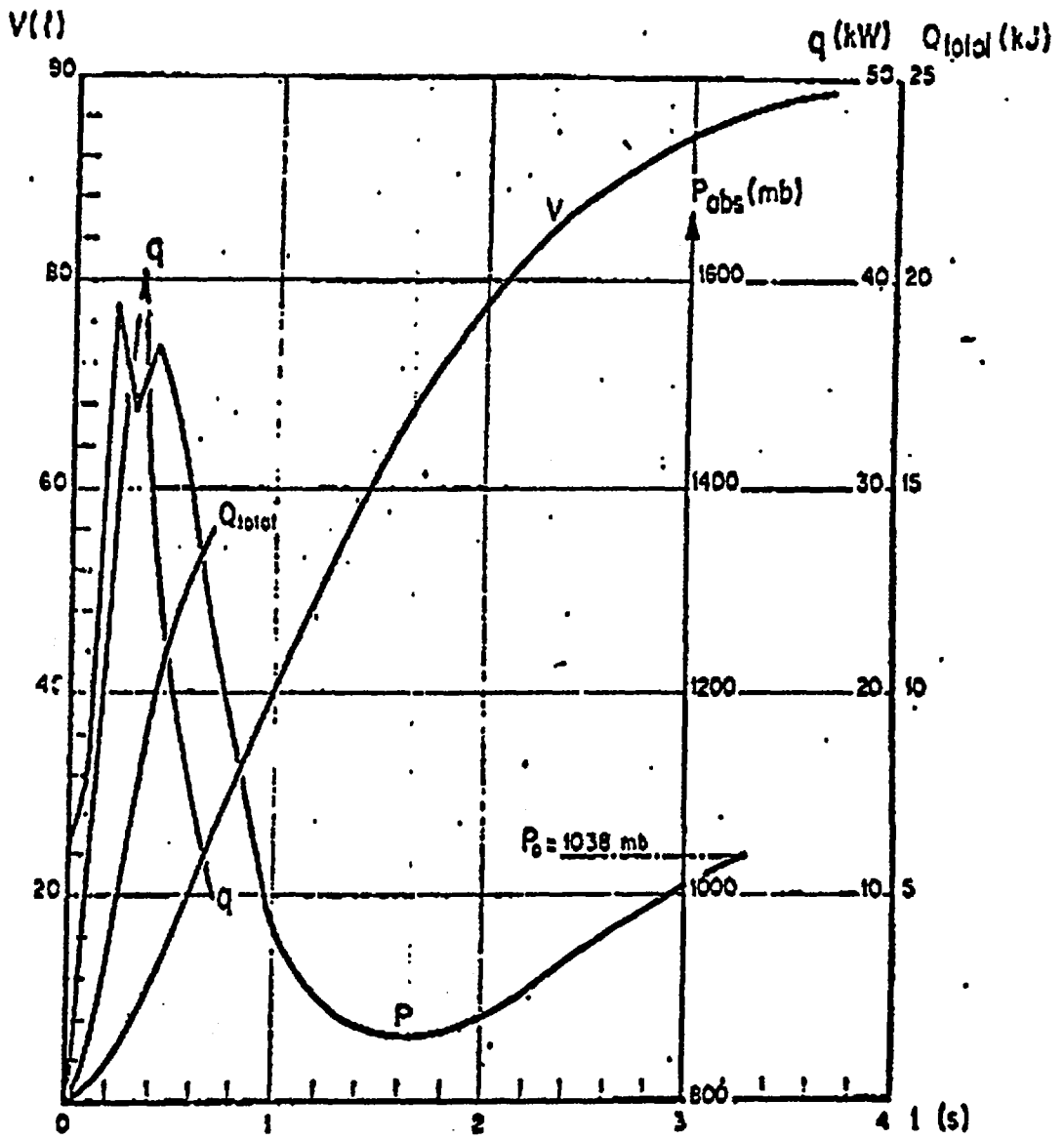


Fig: 4 -  $V_0 = 236 \text{ cm}^3 \text{ H}_2$ , sans ciel.

# MODE OF CONTACT IS IMPORTANT

o Several Type 1 experiments were conducted by breaking the walls locally using an impact hammer

- No explosions occurred, although significant vapor is formed over 1-3 s
- Localized breakage of walls leads to significant bubbling, and relatively gradual mixing with water through "slits" causing vaporization of LH<sub>2</sub>

---> *Such a contact mode can not be expected to result in explosions as the principal criterion of premixing with hot fluid is not present; Grenoble experiments clearly demonstrate this aspect.*

o Type 2 experiment gave rise to explosive interaction between LH<sub>2</sub> & Water

- Overheating and pressurization to 1.5 MPa by breaking the vacuum led to bursting of walls and forced ejection into the bulk coolant
- Excellent premixing followed by localized spontaneous triggering is evidently sufficient to cause explosive thermal energy transfer and vaporization of LH<sub>2</sub> \*\*\*\* No data are given on pressure traces, etc. \*\*\*\*

---> *Contact modes that force premixing will likely lead to explosions*

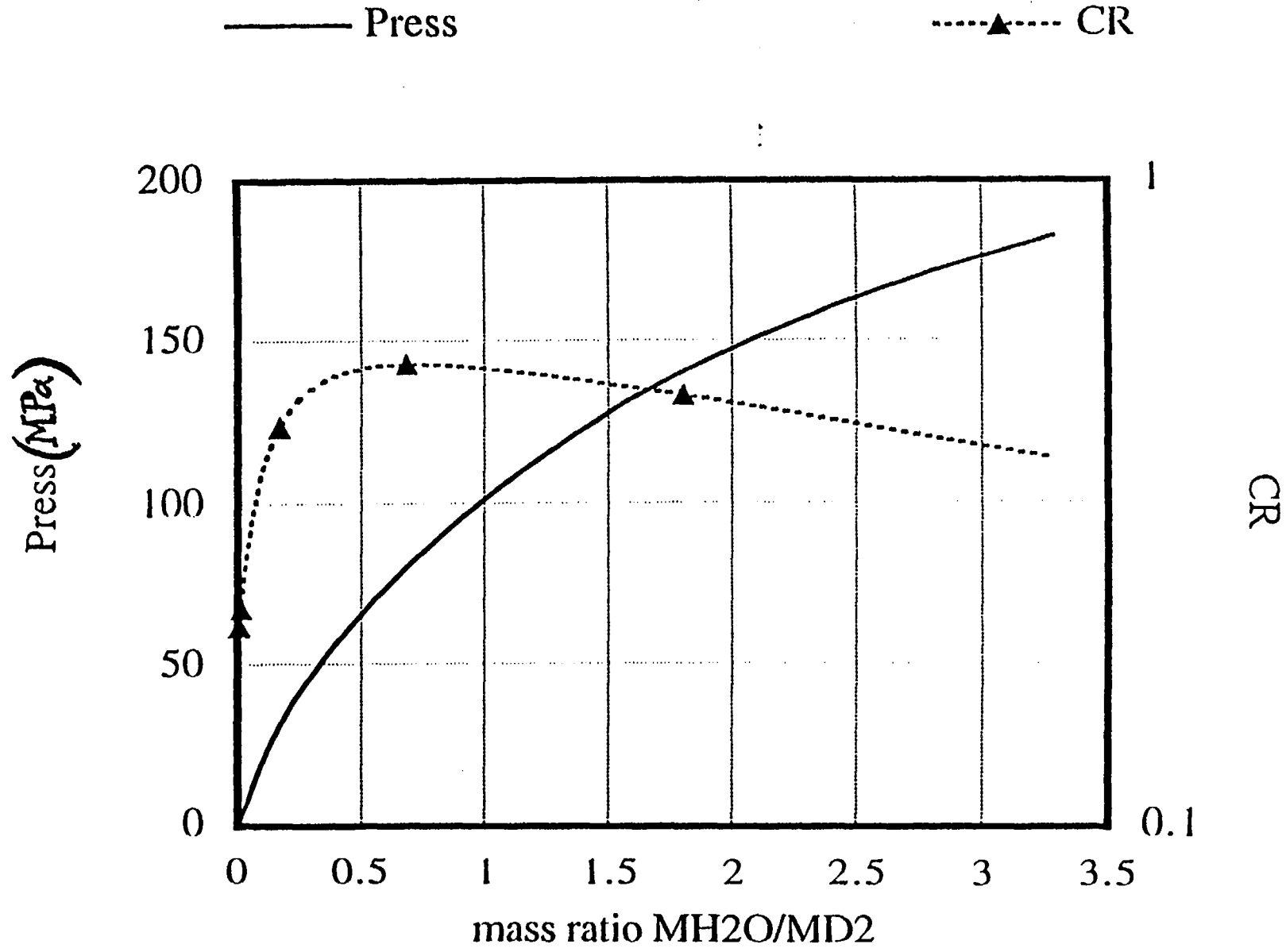
Note: 1 ml of LH<sub>2</sub> at 20.3 K = 55 ml of gas at 20.3 K = 850 ml of gas at 293 K



# ENERGETICS OF EXPLOSIVE LD<sub>2</sub>-WATER REACTIONS

- **MODELING OF ENERGETICS CAN BE DONE MECHANISTICALLY & ALSO USING THERMODYNAMIC MODELS**
  - **But, mechanistic models for modeling cryogenic fluid-water explosions are not well developed**
  - **Thermodynamic models of vapor explosions can be used to provide physically bounding estimates** (but should be used with caution since perfect mixing is assumed and no directional effects are considered)
- **WE HAVE UTILIZED THERMODYNAMIC MODELS** (to evaluate reasonable upper bound estimates of pressurization, and thermal-to-mechanical energy conversion for Advanced Neutron Source beyond design basis accident studies)
  - **Hicks-Menzies model: Essentially adiabatic mixing followed by isentropic fuel-coolant expansion**
  - **Board-Hall model: Essentially simulation of C-J shock front to a given pressure followed by isentropic fuel-coolant expansion**

**Note: Actual properties of LD<sub>2</sub> were utilized; work is preliminary**



Variation of Pressurization (Press) and Conversion Ratio (CR) with Mass Ratio (Hicks-Menzies Approach)