# *Two-phase flow model for energetic proton beam induced pressure waves in mercury target systems in the planned European Spallation Source*

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# *Outline*

- *Motivation*

  ***spallation, some aspects of neutron physics, general remarks, cavitation***

- *The idea of a thermo-hydraulical model,*

  ***gentle introduction into shock-waves (ideal gas)***

  ***general thermo-hydraulics for water***

  ***Equation of states for Hg, proton – Hg interaction***

  ***some new results***

- *Summary and Outlook*

# *Informations:*

ESS General: http://neutron.neutron-eu.net/

ISIS (UK): http://www.isis.rl.ac.uk

SNS (USA): http://neutrons.ornl.gov/

JPARK (Japan): http://j-parc.jp/index-e.html/

**3rd High-Power Targetry Workshop**
**September 10 – 14, 2007, Bad Zurzach, Switzerland**

**organized by the Paul Scherrer Institut, Villigen PSI**

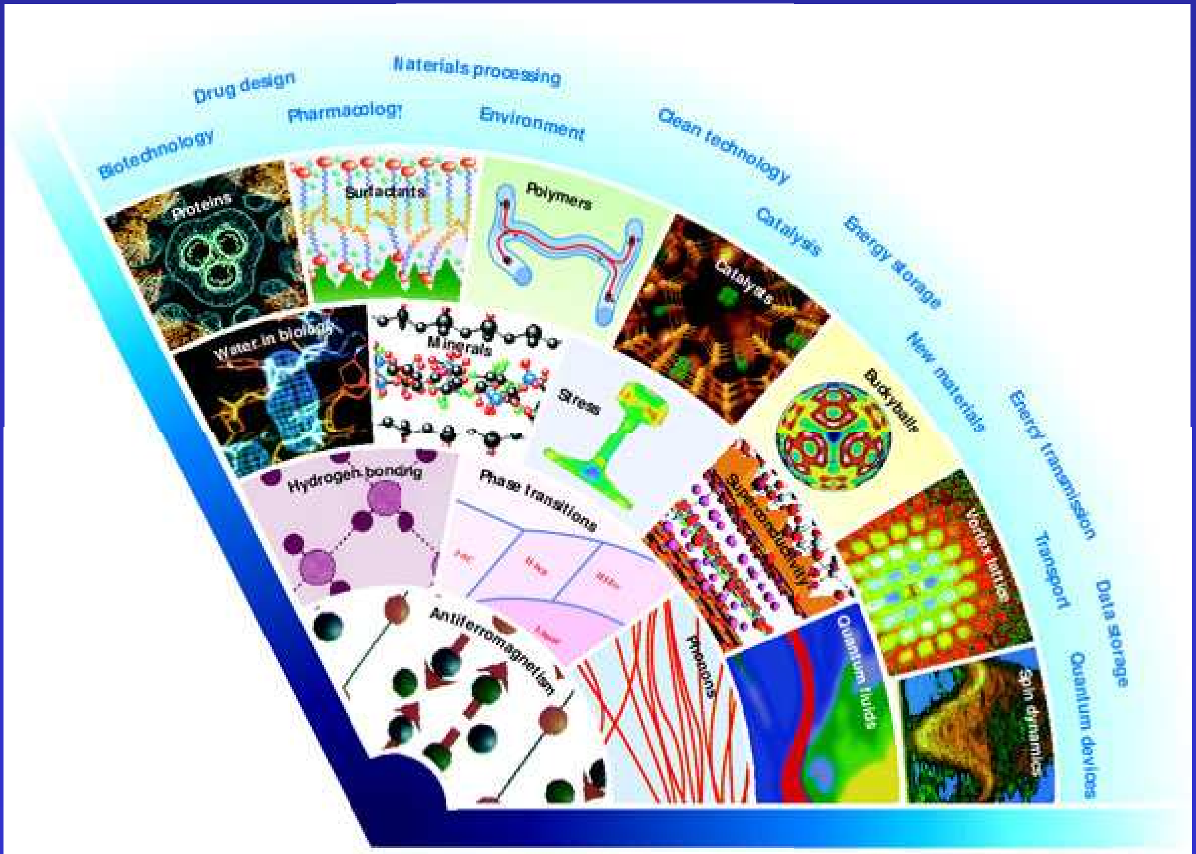
http://asq.web.psi.ch/hptrgts/

(from where some slides/data of the following talk were borowed)

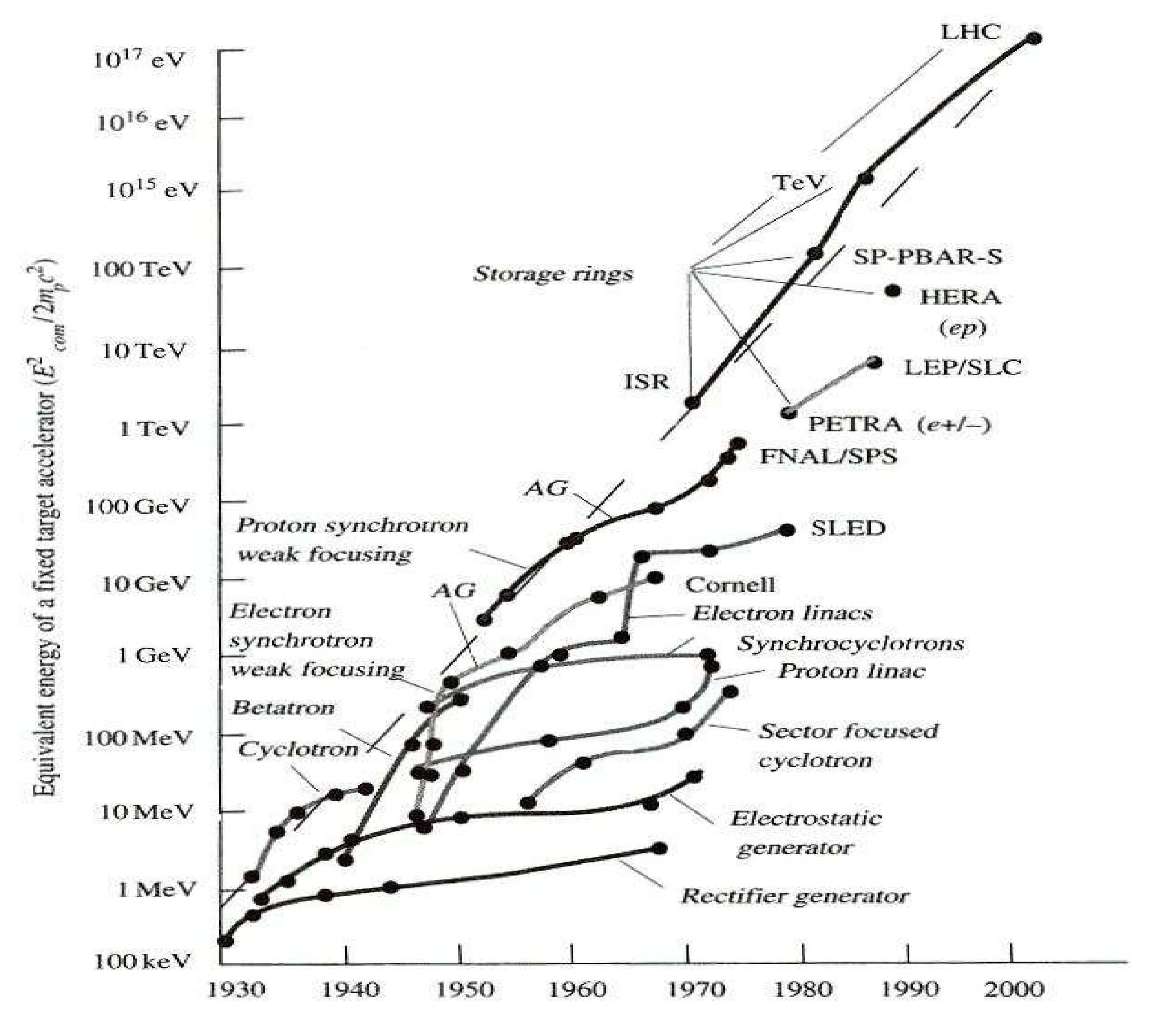
# Motivation I

*Low energy neutrons  scattering is one  fundamental material research method without destruction     (beyond X-ray, and electron scattering)*

*neutrons are enable the structure and dynamics of condensed matter to be probed on a microscopic scale ranging from the subatomic to the macromolecular*



# Motivation II



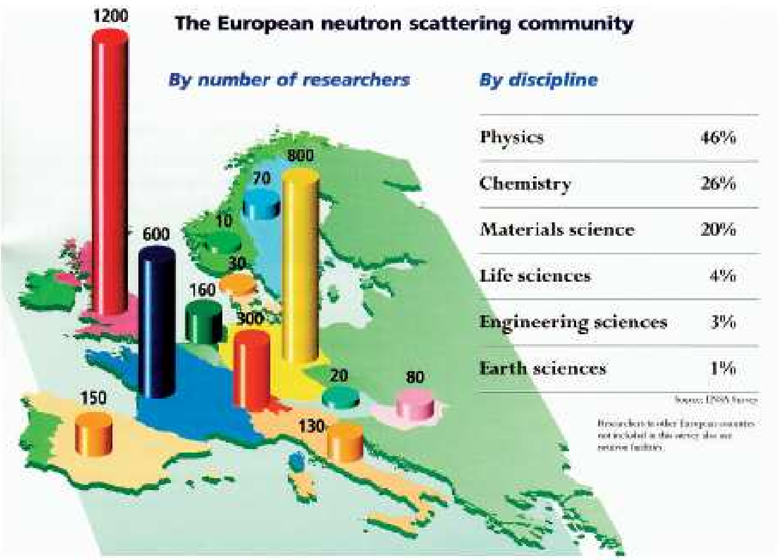
***the produced heat limits the maximal neutron flux in fission sources***

# *Motivation III*

*Relative large european neutron Scientific community*

*Price 0.9 - 1.3 billion (10E9) Euro*

*3 Countries are candidating*
*Spain (Bilbao)*
*Sweden (Lund)*
*Hungary(Debrecen)*
*Hungary is responsible for Thermo-hydraulic, radiation-protection and environmental Studies*



By discipline

| | |
|---|---|
| Physics | 46% |
| Chemistry | 26% |
| Materials science | 20% |
| Life sciences | 4% |
| Engineering sciences | 3% |
| Earth sciences | 1% |

Figure 1: Distribution of neutron users across European countries and scientific disciplines.

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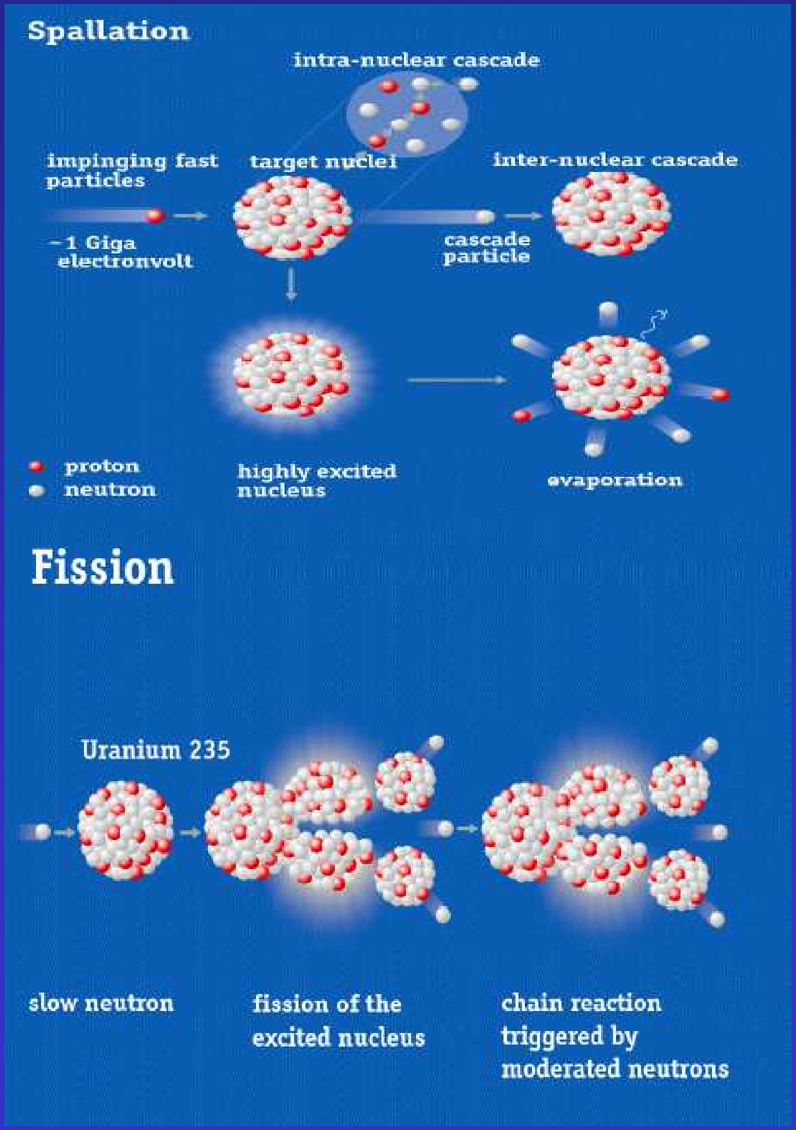
# The Spallation process



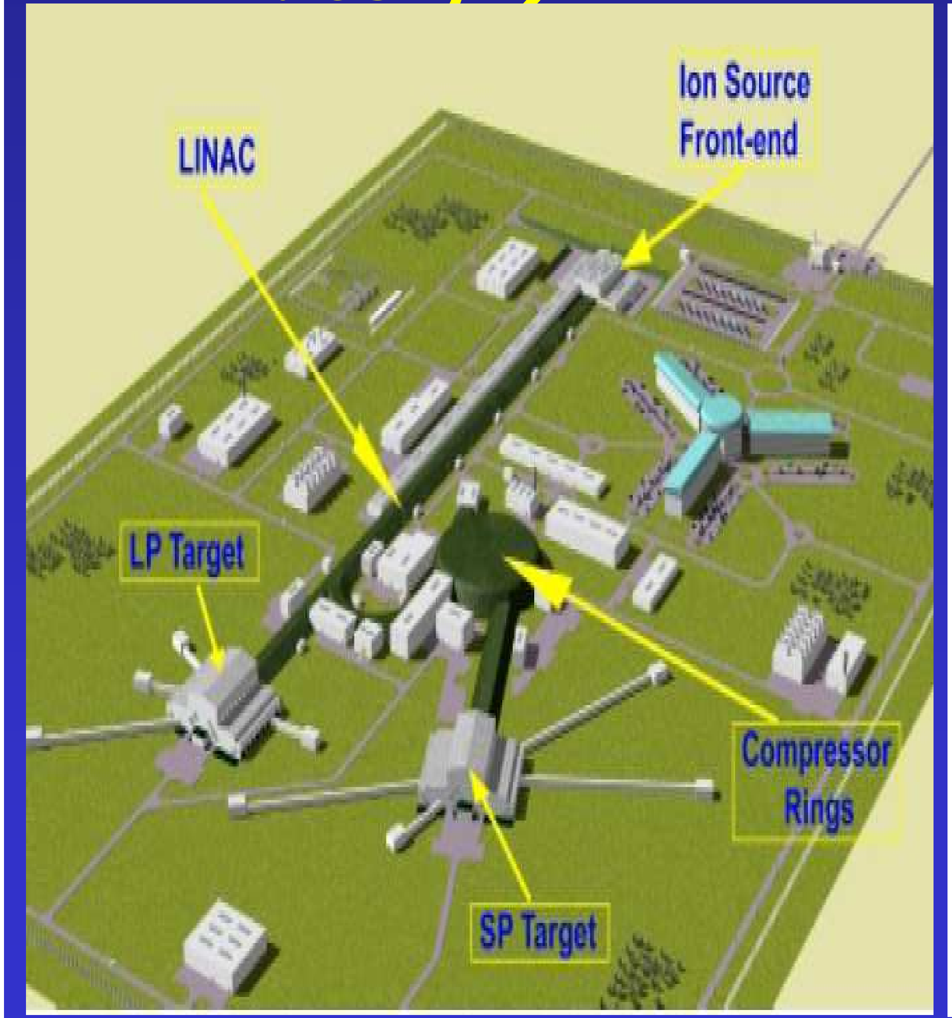
*It is a two step nuclear process, produces about 10 neutrons (and lot more, eg. mesons) without chain-reaction*

*the spectrum of the produced neutrons are favourable than other sources*

*the intensity & shape & length*

*of the neuron pulses are also fortunate*

# A general spallation source (SNS, JSNS,ISIS, *former ESS design*)



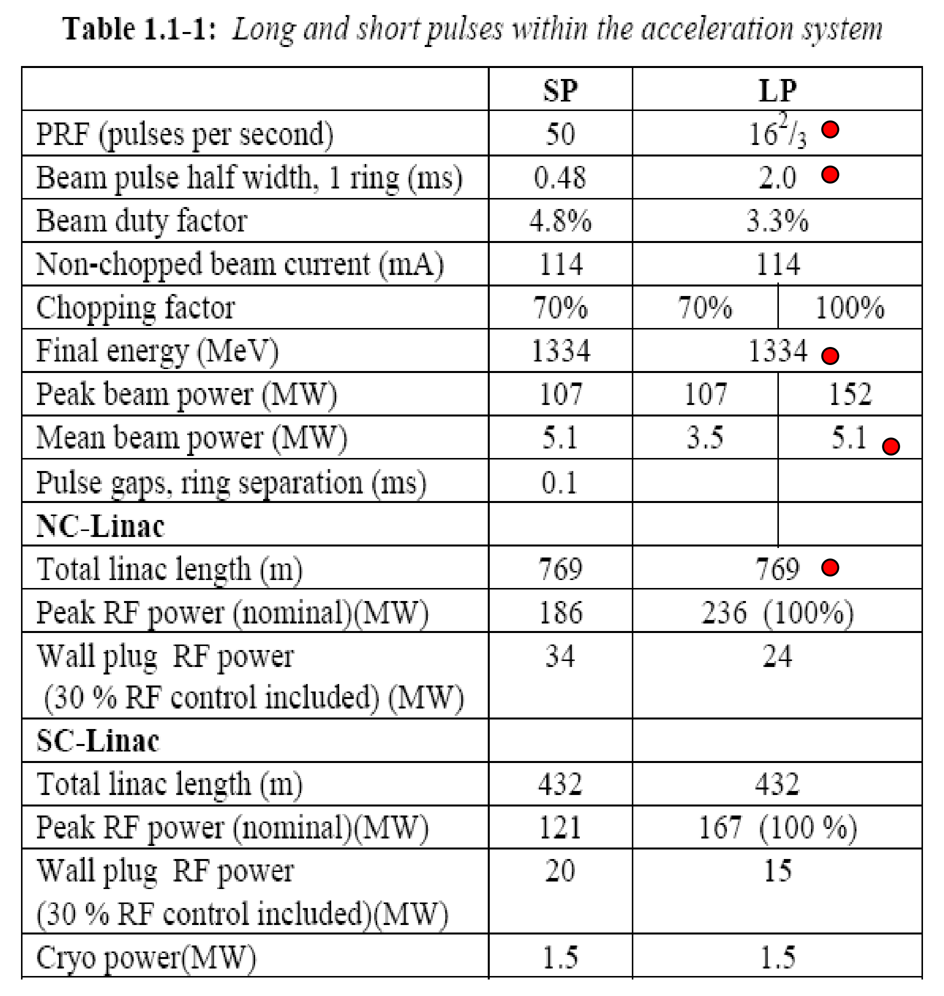
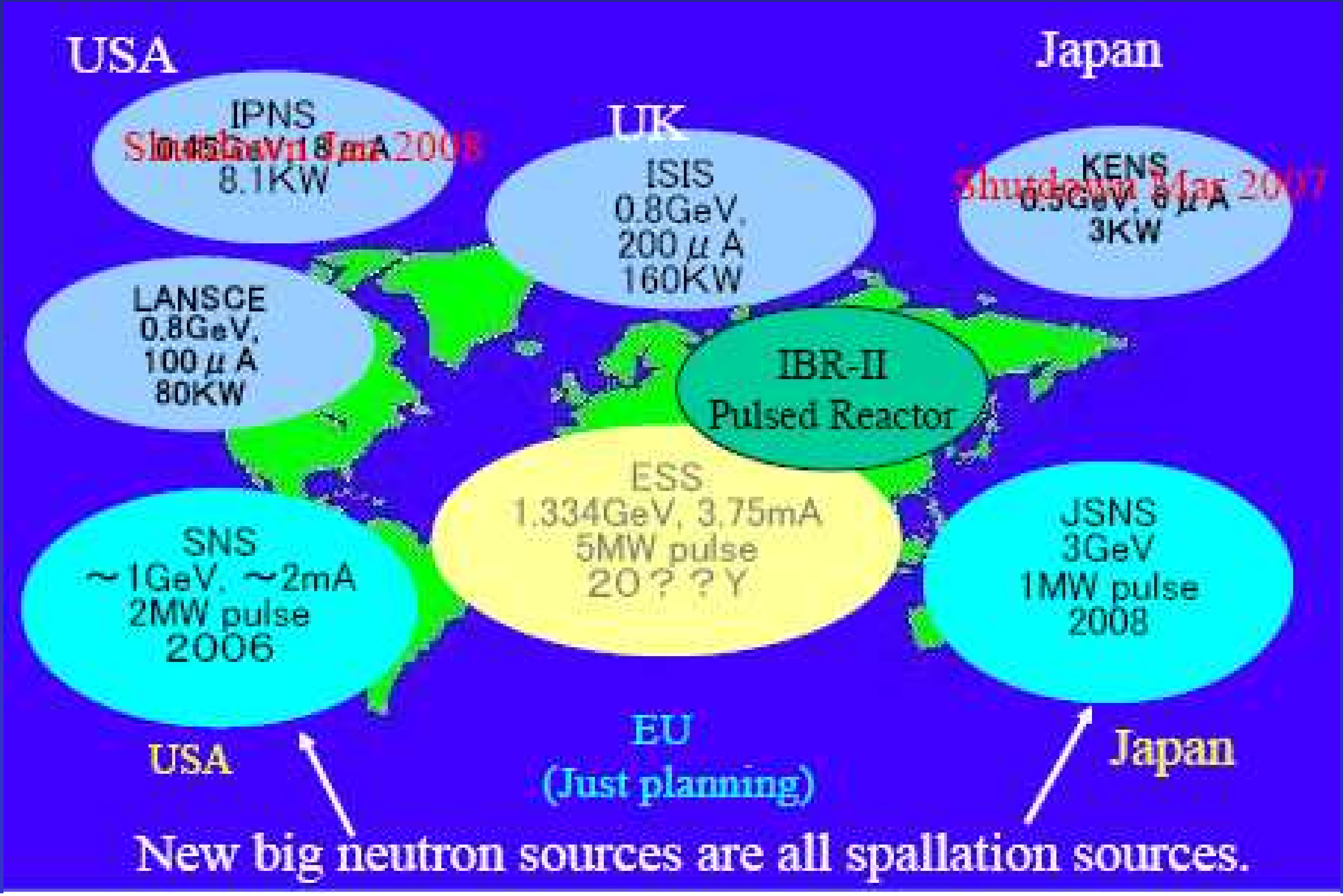


**Table 1.1-1:** *Long and short pulses within the acceleration system*

| | SP | LP | |
|---|---|---|---|
| PRF (pulses per second) | 50 | $16^2/_3$ ● | |
| Beam pulse half width, 1 ring (ms) | 0.48 | 2.0 ● | |
| Beam duty factor | 4.8% | 3.3% | |
| Non-chopped beam current (mA) | 114 | 114 | |
| Chopping factor | 70% | 70% | 100% |
| Final energy (MeV) | 1334 | 1334 ● | |
| Peak beam power (MW) | 107 | 107 | 152 |
| Mean beam power (MW) | 5.1 | 3.5 | 5.1 ● |
| Pulse gaps, ring separation (ms) | 0.1 | | |
| **NC-Linac** | | | |
| Total linac length (m) | 769 | 769 ● | |
| Peak RF power (nominal)(MW) | 186 | 236 (100%) | |
| Wall plug RF power (30 % RF control included) (MW) | 34 | 24 | |
| **SC-Linac** | | | |
| Total linac length (m) | 432 | 432 | |
| Peak RF power (nominal)(MW) | 121 | 167 (100 %) | |
| Wall plug RF power (30 % RF control included)(MW) | 20 | 15 | |
| Cryo power(MW) | 1.5 | 1.5 | |

# Pulsed neutron sources in the world

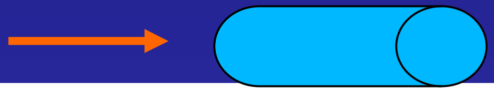


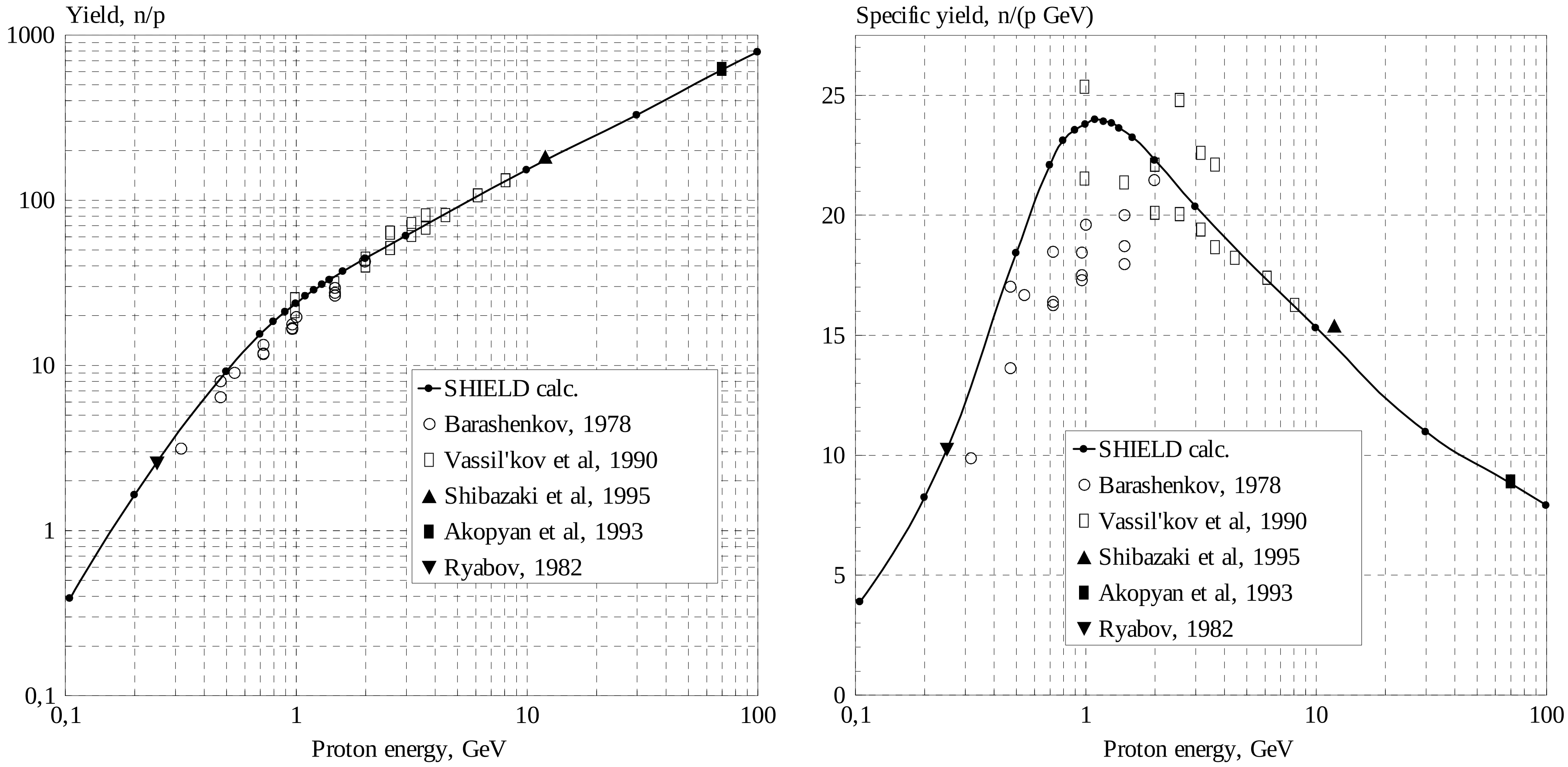
New big neutron sources are all spallation sources.

# Total and specific proton- neutron yield for a 20 cm geometry

answer why

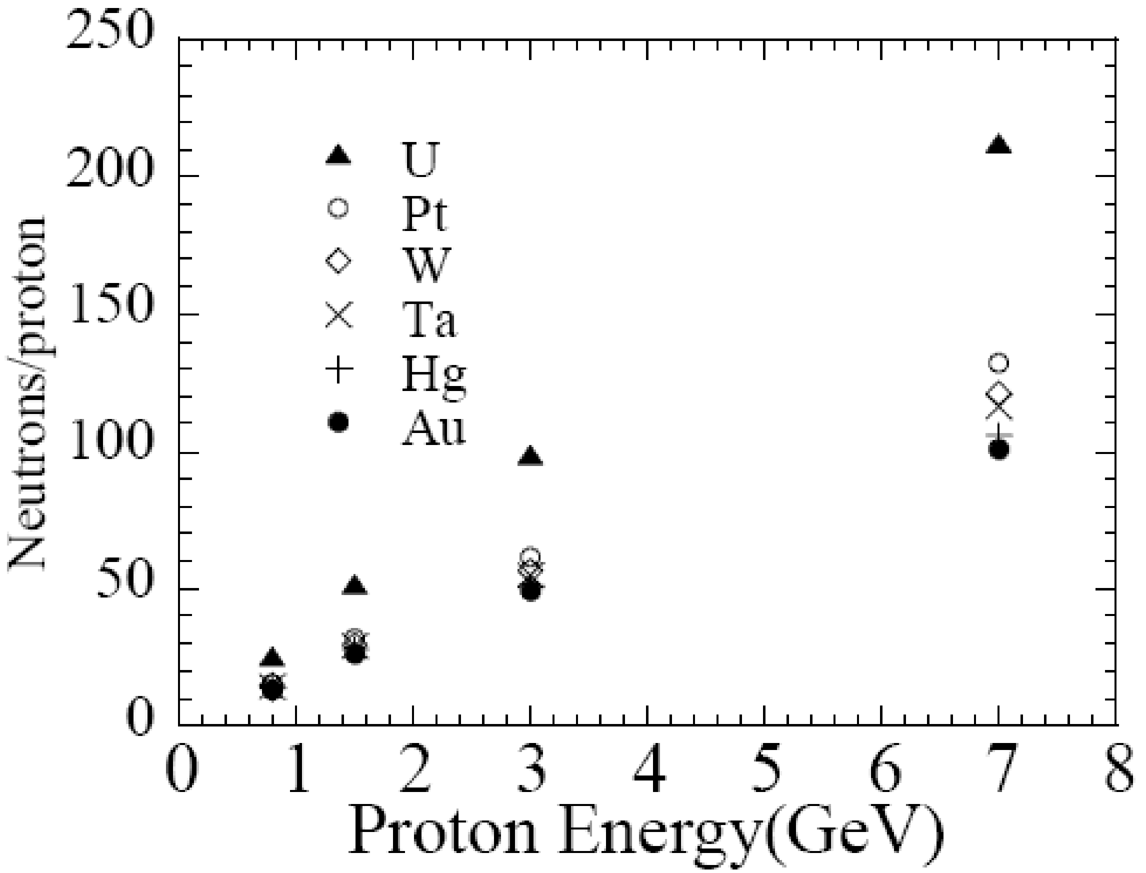
1.3 GeV





# Target materials

Neutron yield vs. proton energy



Neutron yield is not so different in heavy materials other than U producing fission neutron.

We have chosen Hg due to the reason that Hg can be used at higher power than 1 MW.

# *Target Concepts*

(I will show all of them)

- Solid Rotating(tested in Jülich, never worked)
  Fixed(ISIS, UK)

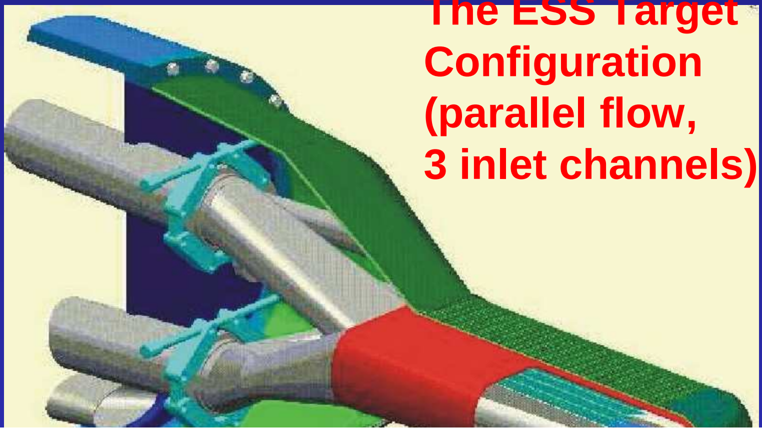
- Liquid Hg(SNS, JSNS, ESS??)
  Lead-Bizmuth Eutectic(SINQ in PSI)

  Major Problems, Shock-Waves, Caviation Dammages, Leakage, unknown life expectancy

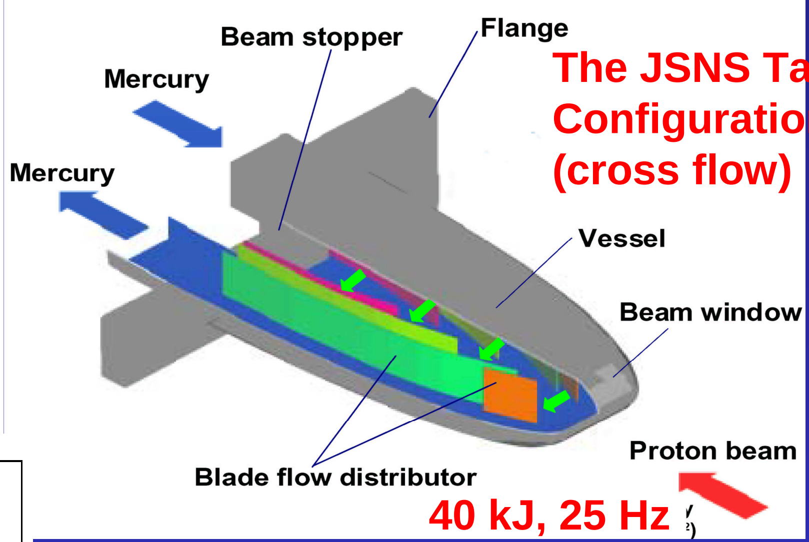
  Solutions: target wall hardening, non-condensable gas injection

ESS target is still in question but Hg is the favorit

# The ESS-SNS-JSNS Hg Target Concepts

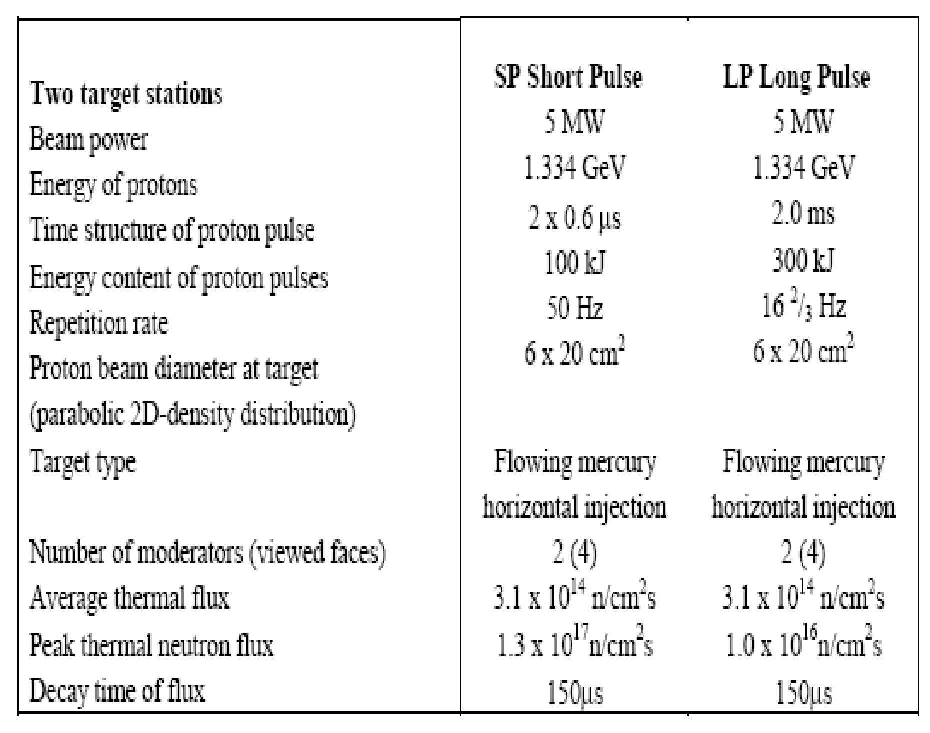


**The ESS Target Configuration (parallel flow, 3 inlet channels)**

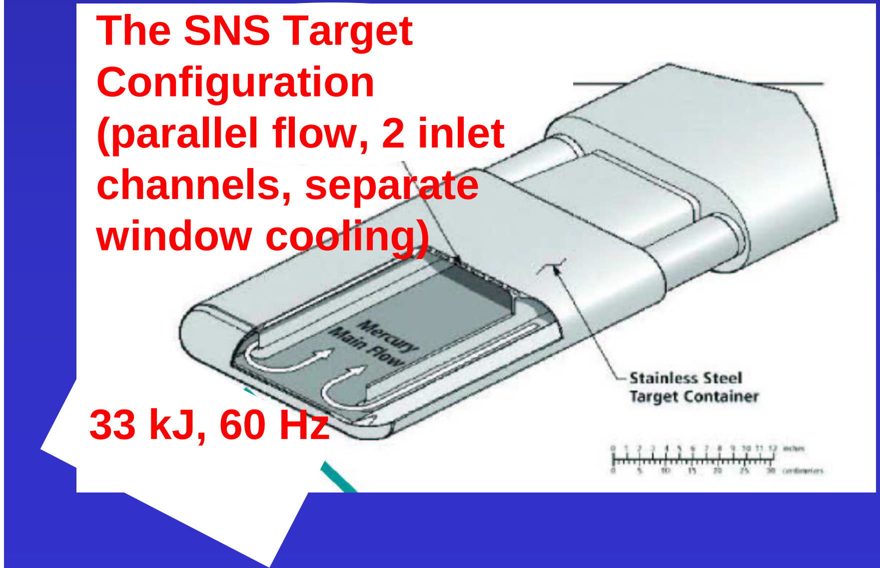


**The JSNS Target Configuration (cross flow)**

**40 kJ, 25 Hz**



| Two target stations | SP Short Pulse | LP Long Pulse |
|---|---|---|
| Beam power | 5 MW | 5 MW |
| Energy of protons | 1.334 GeV | 1.334 GeV |
| Time structure of proton pulse | 2 x 0.6 μs | 2.0 ms |
| Energy content of proton pulses | 100 kJ | 300 kJ |
| Repetition rate | 50 Hz | $16\,^2/_3$ Hz |
| Proton beam diameter at target (parabolic 2D-density distribution) | 6 x 20 cm$^2$ | 6 x 20 cm$^2$ |
| Target type | Flowing mercury horizontal injection | Flowing mercury horizontal injection |
| Number of moderators (viewed faces) | 2 (4) | 2 (4) |
| Average thermal flux | 3.1 x 10$^{14}$ n/cm$^2$s | 3.1 x 10$^{14}$ n/cm$^2$s |
| Peak thermal neutron flux | 1.3 x 10$^{17}$n/cm$^2$s | 1.0 x 10$^{16}$n/cm$^2$s |
| Decay time of flux | 150μs | 150μs |

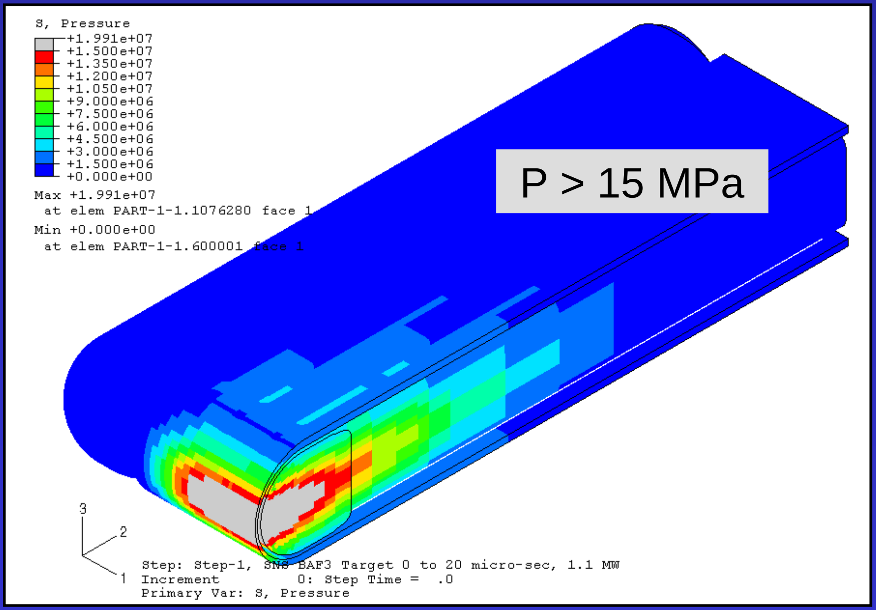


**The SNS Target Configuration (parallel flow, 2 inlet channels, separate window cooling)**

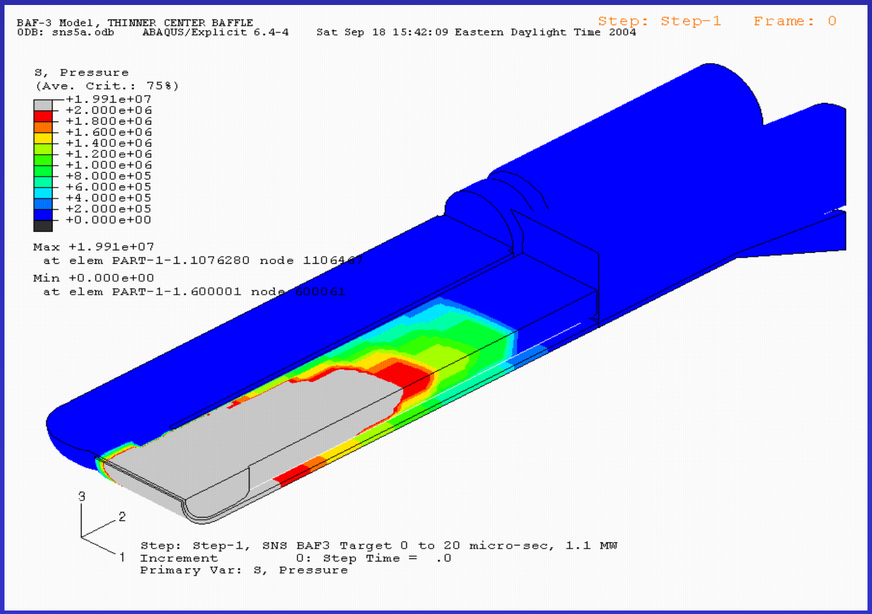
**33 kJ, 60 Hz**

# Simulation techniques applied to SNS mercury target

*Detailed stress and temperature analysis with ANSYS FINE*
*Even two-phase flow thermohydraulical simulations,*
*forcasting large degree of cavitation WELL WELL...*



Mercury pressure right after beam pulse
(P_max = 19.9 MPa @ 1.1 MW)

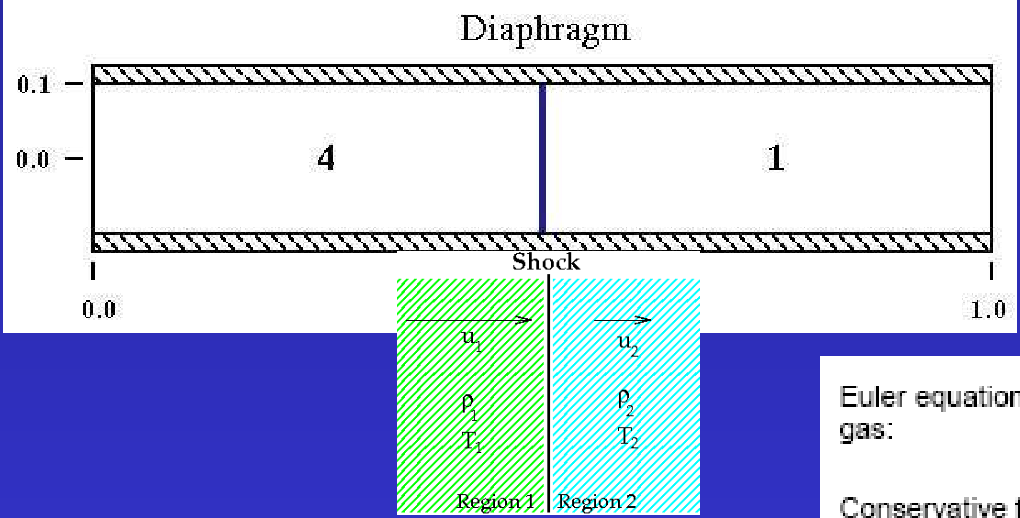


Stress at time of maximum stress
(S_max = 176 MPa @ 0.114 ms)

# Gentle introduction on shock waves, two-phase flow

*Def: a surface of discontinuity propagating in a gas at which density and velocity experience abrupt changes*

→ *we call it a shock wave* *(Zemplén Győző 1905)*



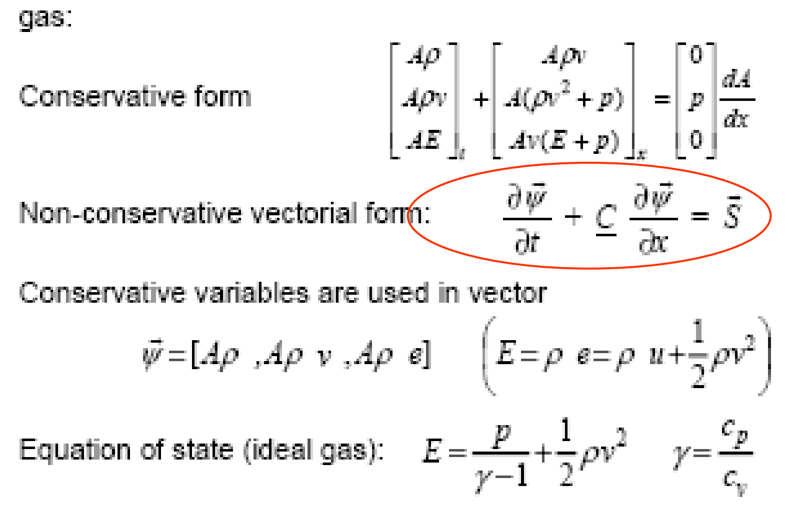
*basic experimental setup*
*(shock tube)*

*mathematical description:*

*conservation laws,*

*continuity, momentum(Euler)*

*energy equation + Equation of state*



Euler equations of single-phase compressible quasi-1D flow of ideal gas:

Conservative form

$$\begin{bmatrix} A\rho \\ A\rho v \\ AE \end{bmatrix}_t + \begin{bmatrix} A\rho v \\ A(\rho v^2 + p) \\ Av(E+p) \end{bmatrix}_x = \begin{bmatrix} 0 \\ p \\ 0 \end{bmatrix} \frac{dA}{dx}$$

Non-conservative vectorial form:

$$\frac{\partial \vec{\psi}}{\partial t} + \underline{C} \frac{\partial \vec{\psi}}{\partial x} = \vec{S}$$

Conservative variables are used in vector

$$\vec{\psi} = [A\rho \ , A\rho \ v \ , A\rho \ e] \quad \left( E = \rho \ e = \rho \ u + \frac{1}{2}\rho v^2 \right)$$

Equation of state (ideal gas): $E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho v^2 \quad \gamma = \frac{c_p}{c_v}$

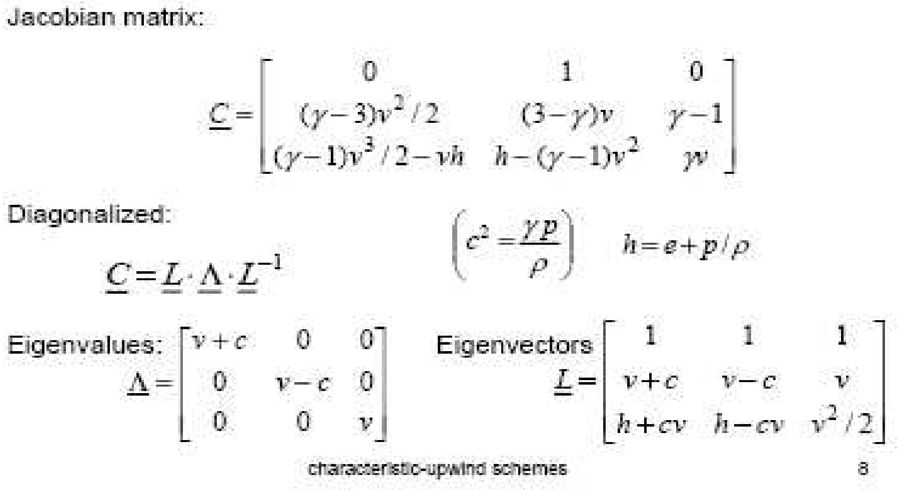
# Gentle introduction on shock waves, two-phase flow

*the measurable physical quantities change in time non-continously, (non-continous solutions for partial differential equations)*

*in a real shock wave physical quantities grow up in approx. 2-4 free mean path of a particle*

*(10^-2 mm at normal p, T, quick phenomena no time for diffusion, heat exchange)*

*the given equations have differents wave solutions with different wave propagation velocities*



Jacobian matrix:

$$\underline{C}=\begin{bmatrix} 0 & 1 & 0 \\ (\gamma-3)v^2/2 & (3-\gamma)v & \gamma-1 \\ (\gamma-1)v^3/2-vh & h-(\gamma-1)v^2 & \gamma v \end{bmatrix}$$

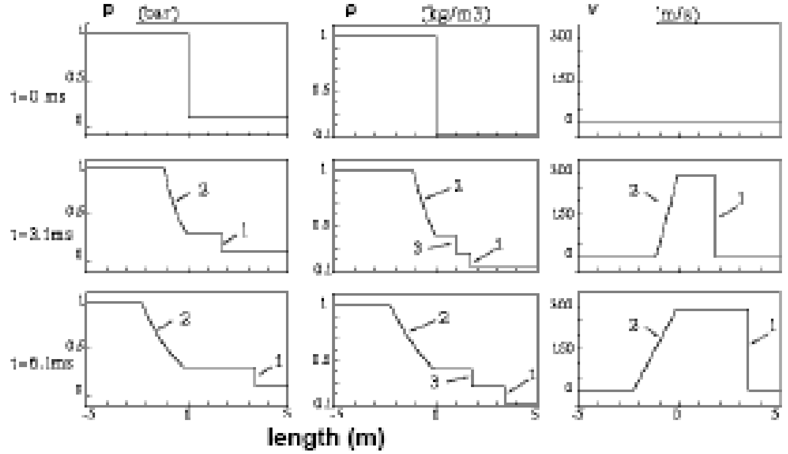
Diagonalized:

$$\underline{C}=\underline{L}\cdot\underline{\Lambda}\cdot\underline{L}^{-1}$$

$$\left(c^2=\frac{\gamma p}{\rho}\right) \qquad h=e+p/\rho$$

Eigenvalues: $\underline{\Lambda}=\begin{bmatrix} v+c & 0 & 0 \\ 0 & v-c & 0 \\ 0 & 0 & v \end{bmatrix}$ Eigenvectors $\underline{L}=\begin{bmatrix} 1 & 1 & 1 \\ v+c & v-c & v \\ h+cv & h-cv & v^2/2 \end{bmatrix}$

characteristic-upwind schemes 8



1- shock wave, 2- rarefaction wave, 3 - contact discontinuity

# *Gentle introduction on shock waves, two-phase flow*

*Shock wave in shock tube for ideal gas:*

*(movies)*

*density wave run_rhot.bat*

*pressure wave run_p.bat*

*speed wave run_v.bat*

# The main problem with shock waves, at high-temperature & high-speed hydrodynamics

fine stuff

Equation of motion: continuity + Euler + energy

Equation of state, (any kind) comes from classical thermodynamics, assume thermal equilibrium e.g. Van der Waals EOS

Not valid!

„Generalized Thermodynamics” (1958) DeGroot

„If the temperature gradient is larget that 1000 K/cm usual thermodynamics does not work”

there is no definition even for temperature & pressure for non-equlibrium thermodynamical system

way out → microscopic theory, local equlibrium in small cells...

# Gentle introduction on shock waves, two-phase flow

- *1D single phase flow can be generalised for 2 phases,* → *averaging over the volume* (void fraction, $\alpha$)

- ***Different models, with diferent number of equ.s***

  *from 3 up to 7 equation models are available, with different physical backgrounds*

$$\frac{\partial \vec{\psi}}{\partial t} + \underline{\underline{C}}\,\frac{\partial \vec{\psi}}{\partial x} = \vec{S}$$

$$\vec{\psi} = (\rho_m, v_m, p_m)$$

$$\vec{\psi} = (\rho_m, \rho_g, \rho_m v_m, \rho_m u_m)$$

$$\vec{\psi} = (\rho_g, \rho_f, \rho_m v_m, \rho_f u_f, \rho_g u_g)$$

*mixture density, velocity, energy is defined*

$$\vec{\psi} = (\rho_g, \rho_f, \rho_g v_g, \rho_f v_f, \rho_g u_g, \rho_f u_f)$$

*we use this one, well tested,*
*single pressure for both phase phases*

$$\vec{\psi} = (\rho_g, \rho_f, \rho_g v_g, \rho_f v_f, \rho_g u_g, \rho_f u_f, 7^{th}\ \text{variable})$$

*could be a two pressure model*

# The numerical scheme of WAHA(our physical model)

$$\frac{\partial \vec{\psi}}{\partial t} + \underline{\underline{C}} \, \frac{\partial \vec{\psi}}{\partial x} = \vec{S}$$

$$\vec{\psi} = ( \, p, \alpha, v_f, v_g, \; u_f, u_g \, )$$

*6 coupled first order partial differential equations,*
*no second-order derivatives,*
*non-conservative variables*

***High resolution, non-dispersive shock capturing first order explicit finite difference schema with second order corrections***

R. Saurel, R. Abgrall, A Multiphase Godunov method for compressible multifluid and multiphase flows, *J. Comp. Physics* **150**, 425-467, 1999.

I. Tiselj, S. Petelin, Modelling of two-phase flow with second-order accurate scheme, *J. Comp. Physics* **136** (2) 503-521, 1997.

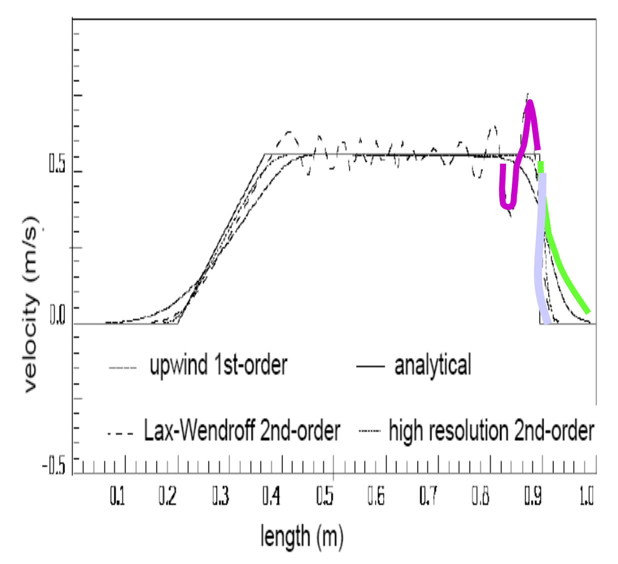
# Idea of the numerical method

- *Hyperbolic partial dif. equ. systems* ⟶ *non-continous solutions*
-
- *(jump initial condition is conserved in time)*
- *Special numerical method is needed*

$$\frac{\partial \vec{\psi}}{\partial t} + \underline{\underline{C}}\,\frac{\partial \vec{\psi}}{\partial x} = \vec{S}$$

*(example: ideal gas shock wave)*

- *Pure 1st order method smears discontinuity*
- *Pure 2nd order creates unphysical oscillations*
- *Mixed method gives physicaly correct answer (flux limiters)*



# *Flow maps, correlations*

**two-phase flows have very complex flow maps**

→ **these are the main uncertanities in the theory**

*we use simplified flow maps*

*stratified, bubbly, droplet flow* *with different correlations*

*Heat-mass, energy, impulse transfer*

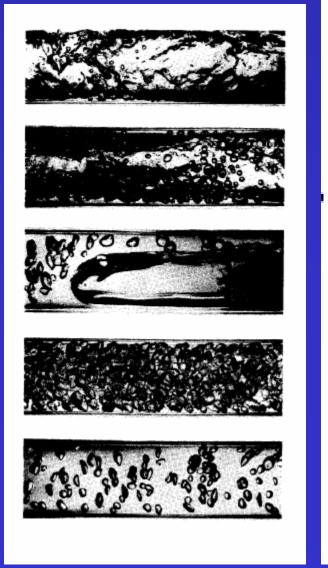
*between phases*

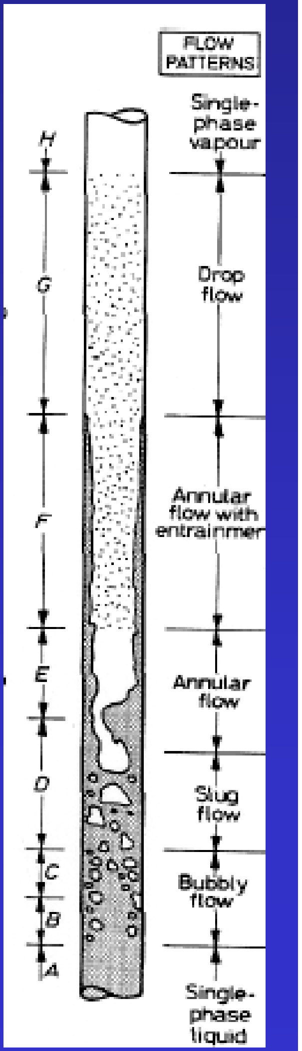
*Wall friction* *steady state/dynamical*

*Interphase friction*

*All can be swtiched on/off for different regimes*

*For steam induced water hammer all correlations are needed*



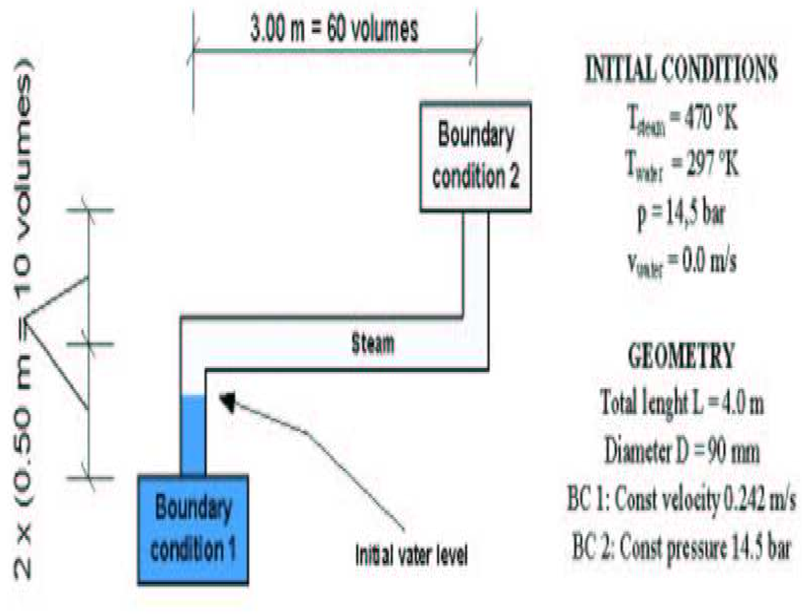


# Our former aim/experience with WAHA

*study of the steam condensation induced water hammer phenomena,*

*the most complex two-phase flow phenomena*

*(experimental setup and the model scheme in numerical simulation)*



INITIAL CONDITIONS

$T_{steam} = 470\ °K$

$T_{water} = 297\ °K$

$p = 14{,}5$ bar

$v_{water} = 0.0$ m/s

GEOMETRY

Total lenght L = 4.0 m

Diameter D = 90 mm

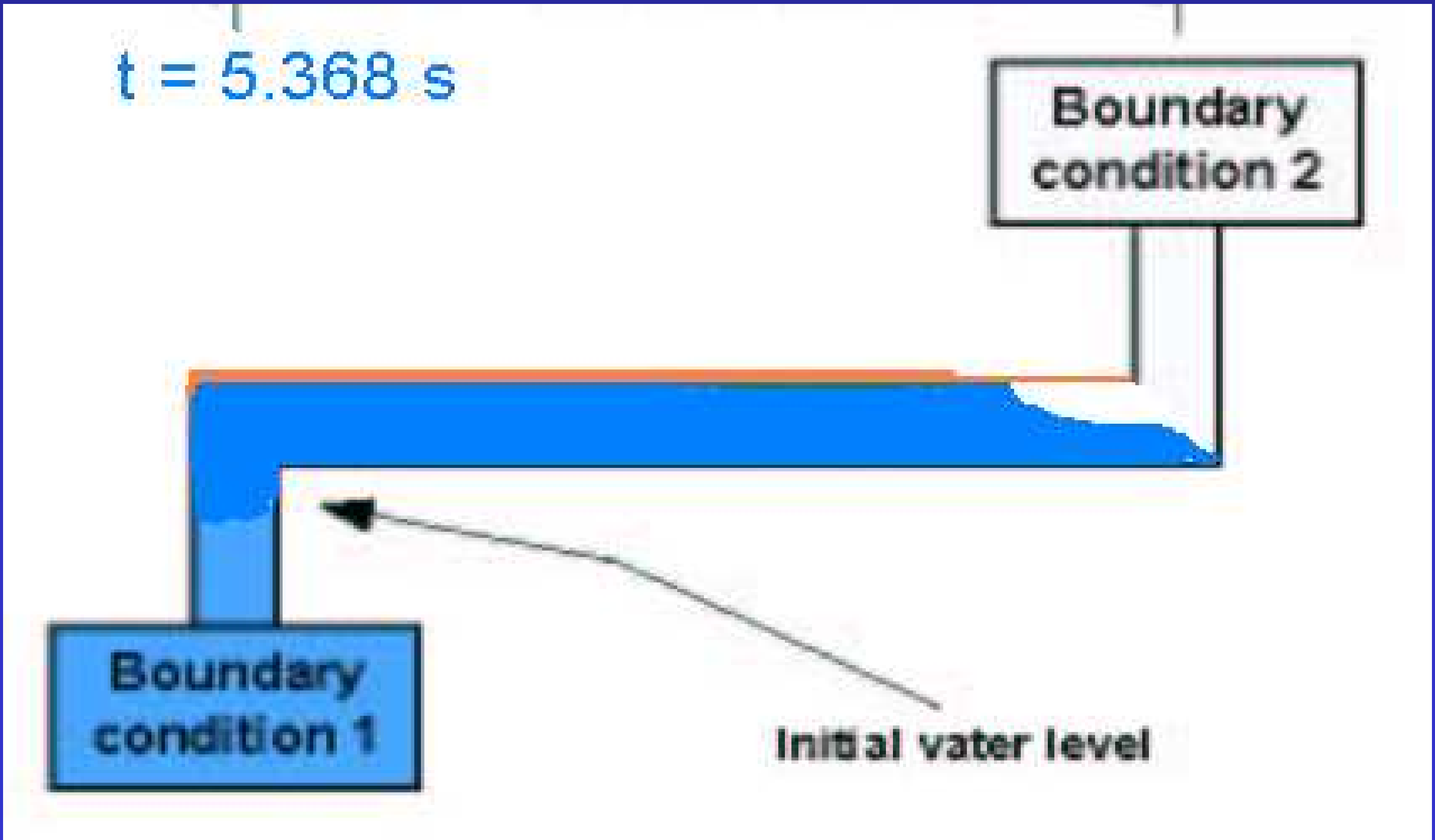
BC 1: Const velocity 0.242 m/s

BC 2: Const pressure 14.5 bar

**Tube volume 12 litre**

# A possible mechanism for steam condensation induced water hammer

*(some figures)*



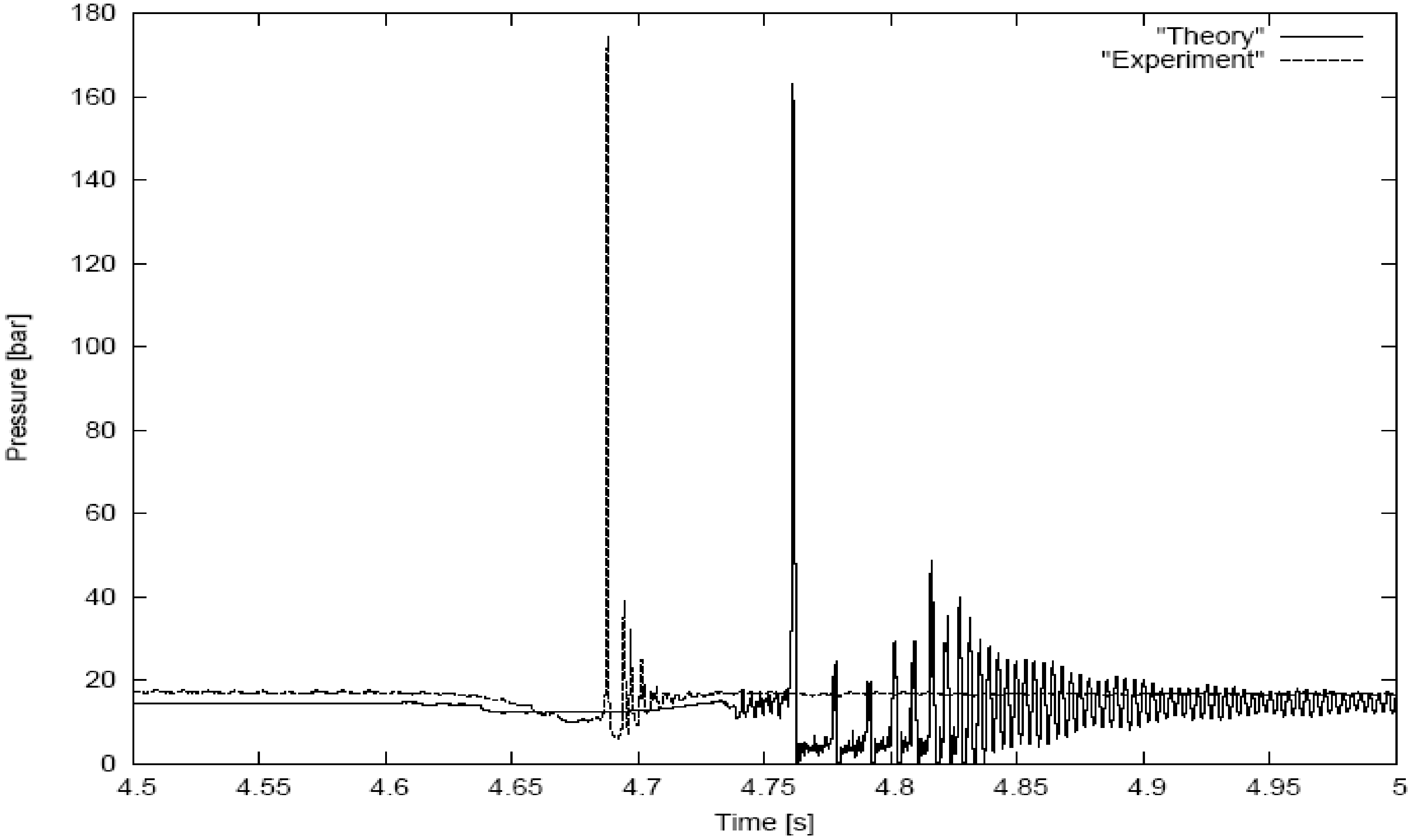
# A possible mechanism for steam condensation induced water hammer (animation)

The whole physical process: kfki.avi

a slow replay of the water hammer: kfki_det.avi

# Analysis of the pressure peaks

*(all the correlations/know hows are needed)*



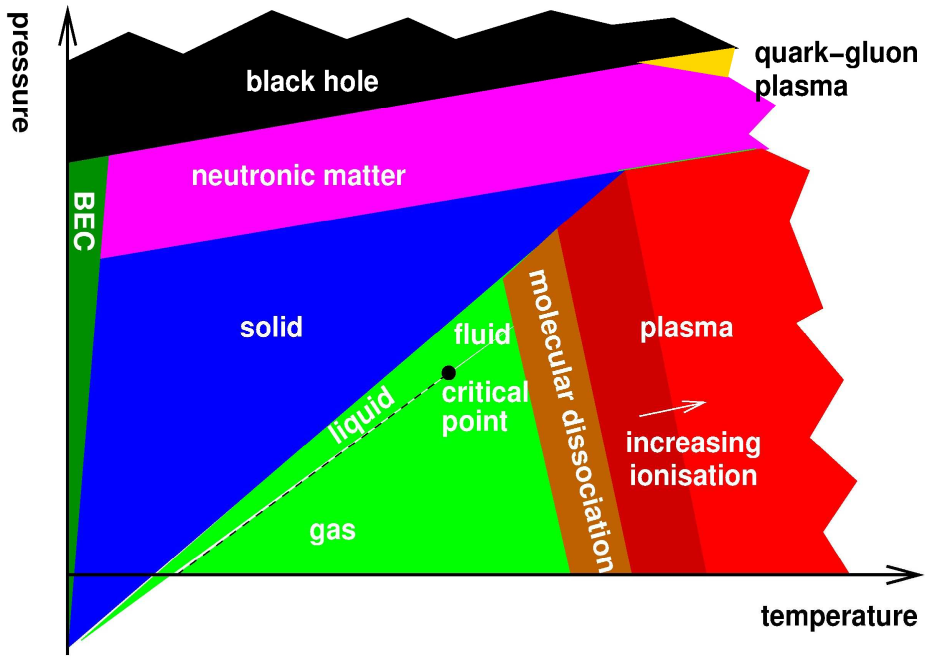
# Idea, use the modified 6equ. model for proton – Hg interaction

- Basicaly two new points
- Not water but mercury (new & complete liquid- steam table), equation of state (EOS) (Subbotin correlation, surface tension, heat conduction, viscosity is known)
- Periodic driving from absorbed proton pulses, a new source term in both energy equations

# How matter looks like

*(On the way of an EOS for Hg)*

Structure of the equation of state



Details depend on the material composition.

*3 different type of EOS*

$\rho(p,T)$ *based on:*

*1) microscopic, classical methods, particles in potential and/or quantum mechanical eg. density functional*

*2) mesoscopic calculations*

*averaging of distribution functions*

*3) macroscopic, fenomenological,*

`http://public.lanl.gov/dswift`

# Different EOS for liquid-gas phase

$PV = nRT$ *ideal gas No phase transition 1834*

$$\left(P + a/V^2\right)(V - b) = RT$$ *Van der Waals 1873*

$$a = 3P_c \cdot V_c^2 \quad b = V_c/3.$$

- Berthelot

$$P = \frac{nRT}{V - nb} - \frac{n^2 a}{TV^2} = \frac{RT}{V_m - b} - \frac{a}{TV_m^2}$$

- Dieterici

$$P = \frac{nRTe^{-\frac{an}{RTV}}}{V - nb} = \frac{RTe^{-\frac{a}{RTV_m}}}{V_m - b}$$

- Redlich-Kwang

$$P = \frac{nRT}{V - nb} - \frac{n^2 a}{\sqrt{T}V\left(V - nb\right)} = \frac{RT}{V_m - b} - \frac{a}{\sqrt{T}V_m\left(V_m - b\right)}$$

$$\left(P + \frac{a(T)}{V(V + b)}\right)(V - b) = RT$$

*Soave-Redlich-Kwang 1972*

$$\left(P + \frac{a(T)}{V(V + b) + b(V - b)}\right)(V - b) = RT$$ *Peng-Robinson 1976*

$$\left(P + \frac{a(T)}{\left[V - b_1(T)\right]\left[V - b_3\right]} - \frac{e}{\left[V - b_1(T)\right]^2\left[V - b_3\right]}\right)\left[V - b_1(T)\right] = RT$$

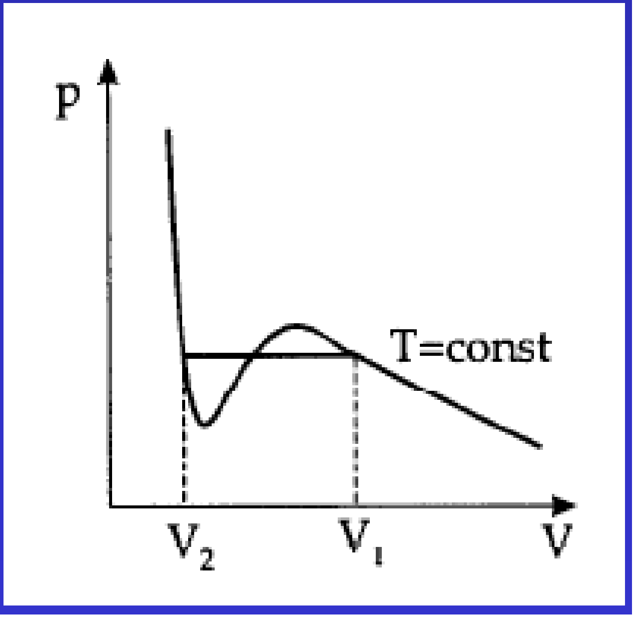
*Shell Research and Technology Center (cubic-4G) (oil industry)*

**Basicaly third order polinom fits**

# How to create a steam table for Hg

For standard 2 phase-flow calculation a 6-fold table is needed:
T (K), p (Pa), $\rho$_vap (kg/m^3), u_vap (J/kg), $\rho$_liq (kg/m^3), u_liq (J/kg)

from the EOS
the smallest and the largest real roots
of the third order polinom at a given T
and P are proportional with the inverse of
the liquid and steam densities,
Maxwell construction for saturation pressure



# How to create a steam table for Hg

to calculate the internal energies is a bit more difficult

for liquid:
just integrate

$$dU = C_V dT + \left[T\left(\frac{\partial P}{\partial T}\right)_V - P\right] dV$$

additional experimental data (fitted function of) specific heat

$$C_p = C_v - T\left(\frac{\partial V}{\partial T}\right)_P^2 \left(\frac{\partial P}{\partial V}\right)_T.$$

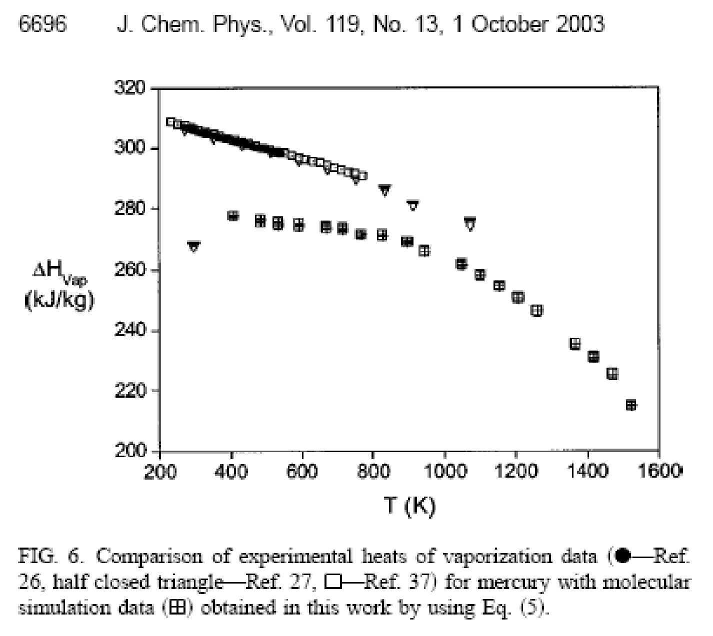
$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)$$

thermal expansion coefficients
(fitting of experimental data)

This can be solved by Maple package ☺

for gas phase:
just substract
vaporization enthalpy

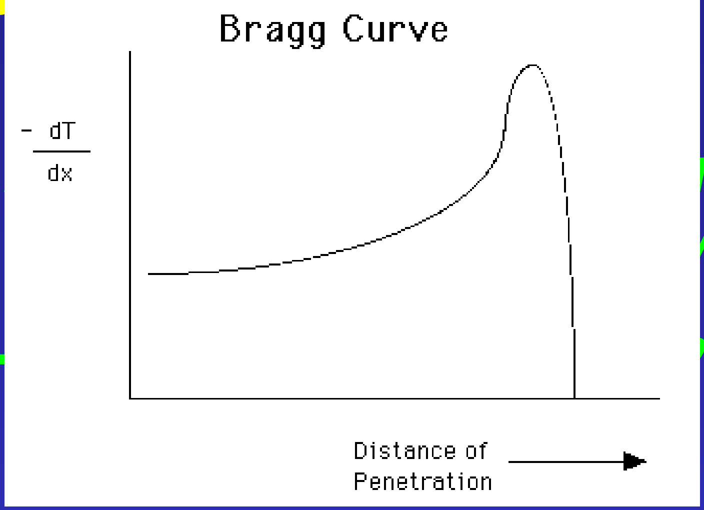
just fitting experimental data



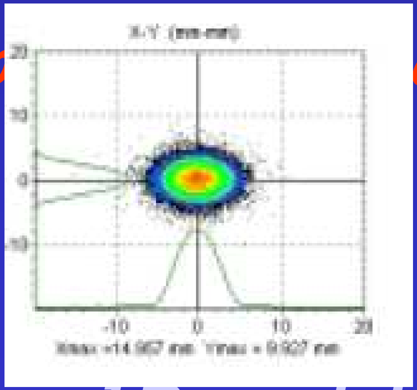
6696 J. Chem. Phys., Vol. 119, No. 13, 1 October 2003

FIG. 6. Comparison of experimental heats of vaporization data (●—Ref. 26, half closed triangle—Ref. 27, □—Ref. 37) for mercury with molecular simulation data (⊞) obtained in this work by using Eq. (5).

# Proton beam-Hg target interaction



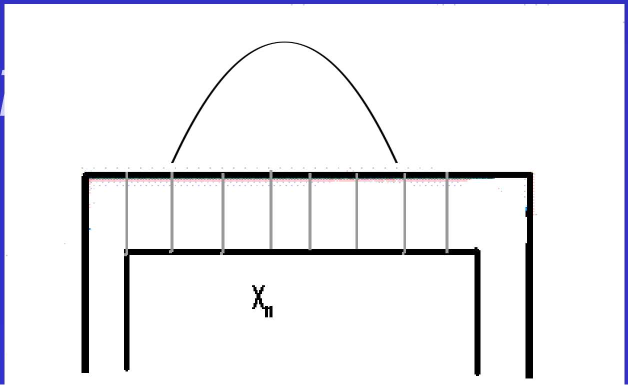
- Accurate e gg peak) of proton in Hg can with FLUKA, MARS, GEANT etc. le heat deposition



- beam p dratic (measured)

$$\rho(x,y) = \frac{3\lambda}{2\pi ab}\left[1-\frac{x^2}{a^2}-\frac{y^2}{b^2}\right]^{½}$$

- We have 1D model only



# The new source terms

- We consider proton beam-Hg interaction as a periodic sudden heat shock in the *energy* equation of the liquid and gas phase

$$\frac{\partial \vec{\psi}}{\partial t} + \underline{\underline{C}}\, \frac{\partial \vec{\psi}}{\partial x} = \vec{S}$$

$$\frac{\partial A(1-\alpha)\rho_f u_f}{\partial t} + \frac{\partial A(1-\alpha)\rho_f u_f v_f}{\partial x} - p\frac{\partial A\alpha}{\partial t} + p\frac{\partial A(1-\alpha)v_f}{\partial x} = A\left(Q_{if} - \Gamma_g h_f^{*} + v_f F_{f,wall}\right) + E_{f,pulse}(x,t$$

$$\frac{\partial A\alpha\rho_g u_g}{\partial t} + \frac{\partial A\alpha\rho_g u_g v_g}{\partial x} + p\frac{\partial A\alpha}{\partial t} + p\frac{\partial A\alpha v_g}{\partial x} = A\left(Q_{ig} + \Gamma_g h_g^{*} + v_g F_{g,wall}\right) + E_{g,pulse}(x,t)$$

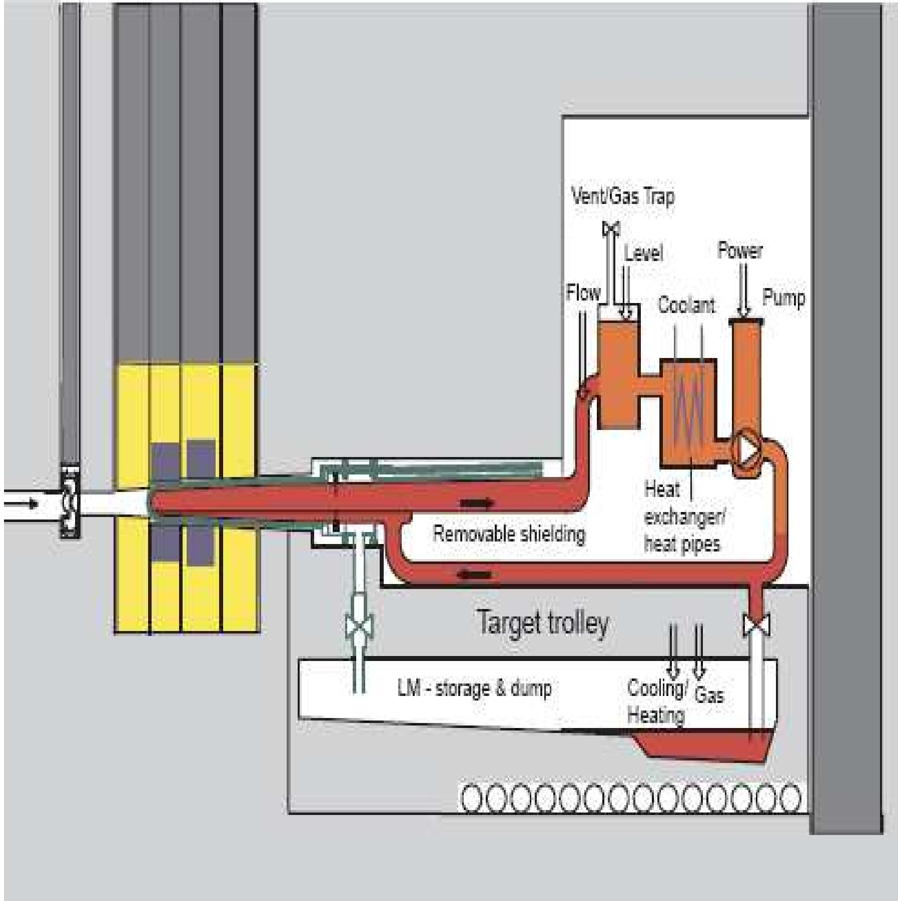
$$E_{g,pulse}(x,t) = \frac{\rho_g\alpha}{\rho_m} E_0 sin^2\left[\frac{\Pi t}{\tau}\right]\left(1-(x/x_s)^2\right)$$

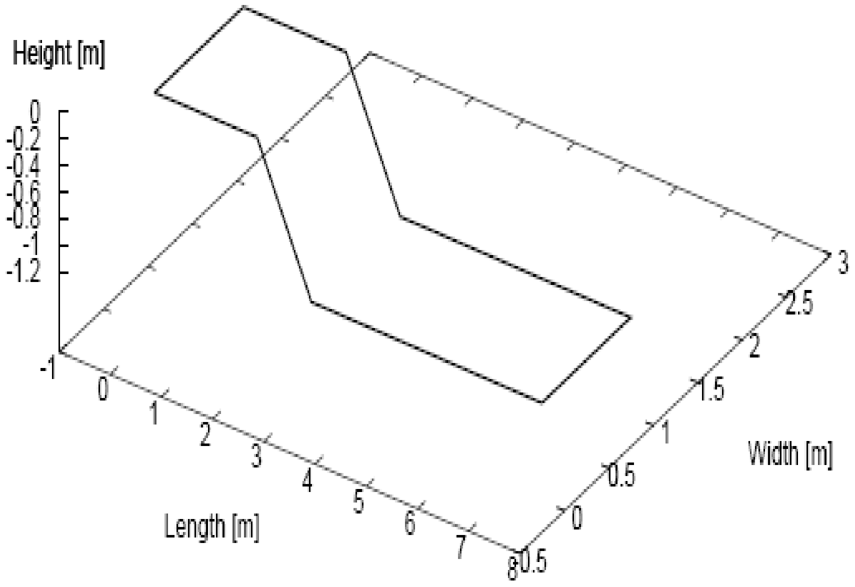
$$E_{f,pulse}(x,t) = \frac{\rho_f(1-\alpha)}{\rho_m} E_0 sin^2\left[\frac{\Pi t}{\tau}\right]\left(1-(x/x_s)^2\right)$$

*continuity, momentum equations will not be changed*

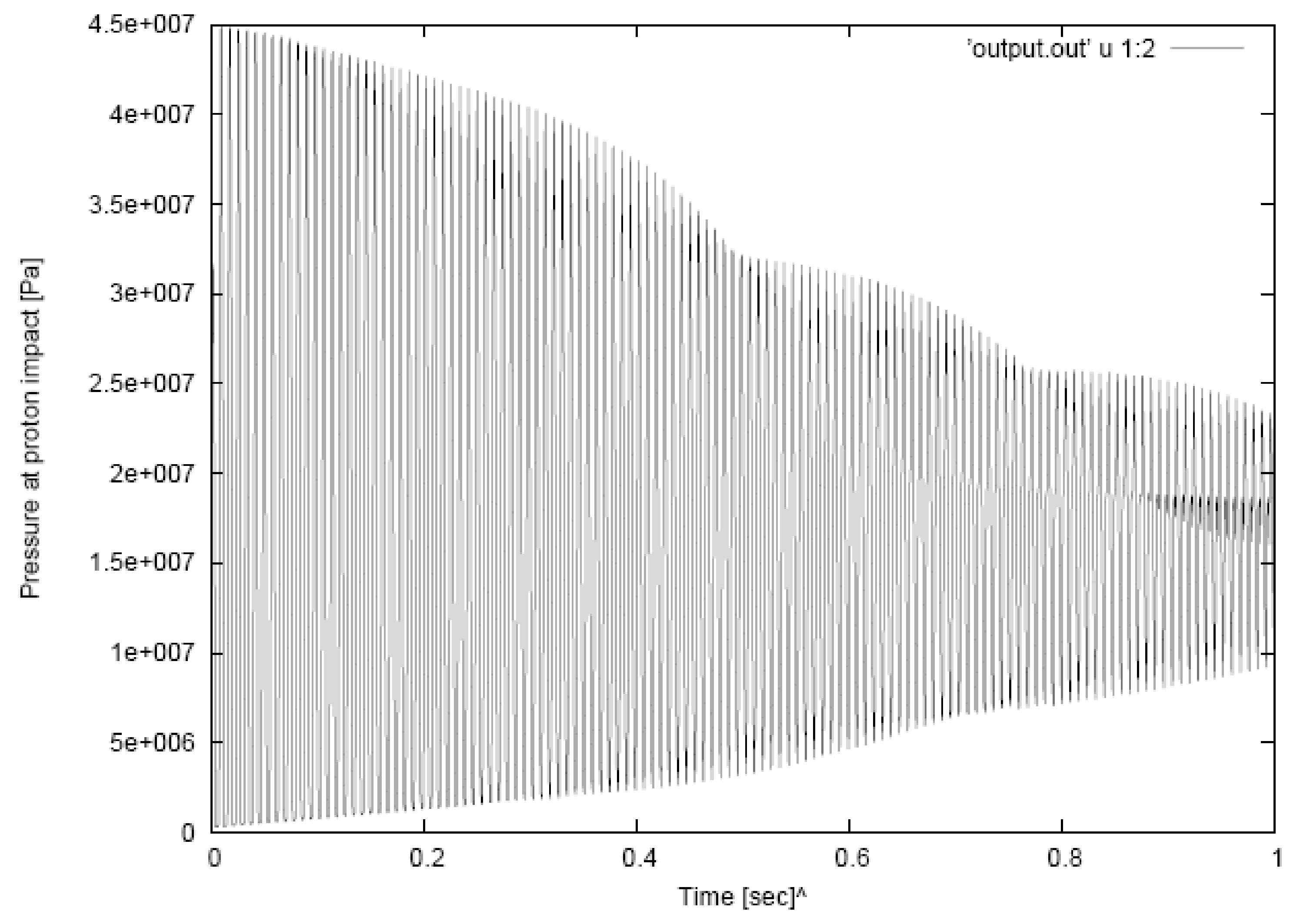
# The scematic scheme of the target

*No sophisticated 3D model, like Fluent, Ansys of CFX NO ENGINEERING*
*But better phyiscs for boiling-condensation, 2 phase flow*





# Our first results



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# *Summary and Outlook*

*we shortly presented the planned ESS apparatus, and the proton-mercury target system*

*gave a short/gentle introduction into shock waves/2phase flow ☺*

*introduced the WAHA3 model, which is feasible to describe shock waves, quick transients in two phase-flows*

*presented a model which is hopefully a good choice to understand some new physics in proton-Hg system*

*further work is in progress to clear out the dark points and present reasonable results*

I.F. Barna European Physical Journal B,
Cite as: arXiv:0805.3618v1 [cond-mat.other]

*There are liquid-metal (eq. Li) or liquid helium cooled systems as well… ☺*
*(work for the next 20-30 years)*

# Thank you for your attention!

Questions, comments, remarks?...