Modeling of heat and hydrodynamic processes in the big uranium target “BURAN” under the action of high-energy ions

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Abstract. This paper is devoted to the analysis of heat transfer, hydrodynamic and acoustic processes induced by high-energy particles irradiating the big uranium target “BURAN”. The generation of heat and acoustic waves by relativistic ion beams is studied numerically. Energy transfer between irradiated target and ambient atmosphere was analyzed with different models. The study provides a basis for development of the new acoustic method for analysis of ion beam energy deposition and its further redistribution in the bulk of a target.

1. Introduction
Atomic power production as an alternative to the conventional power production via burning of organic fuel is quite attractive. The important reasons hampering its wide development in the world are the problems of safety, nuclear waste storage, utilization of spent nuclear fuel, as well as the involvement of natural and depleted uranium and thorium, in the energy production cycle. The idea of utilizing accelerated particle beams in nuclear power production has been discussed since the 1950s [1, 2, 3]. Among such concepts is the accelerator-driven system (ADS) representing a subcritical fast reactor with an external source of neutrons. The concept of accelerator driven systems implies after-burning of nuclear fuel with the help of neutron fluxes produced in fission of natural and depleted uranium, thorium and other heavy elements. This concept is attractive in a number of ways: safe operation of ADS systems, transmutation of minor actinides in nuclear waste, short (as compared to fast reactors) cycle of fissionable materials recovery, etc. [4, 5, 6, 7, 8]. With increasing beam energy and corresponding hardening of the secondary neutron spectrum, one may hope to utilize spent nuclear fuel for power production [9, 10]. Thus, the interest in investigations in this field is grounded.

Nowadays, a special station for investigations in the field of nuclear power production at extracted beams of the NICA accelerator complex is under development at the Joint Institute for Nuclear Research. The new concept of ADS power production with light ion beams of intermediate energies [11] taking into account the energy spent for particle beam acceleration is
much less demanding to the accelerator part of the ADS concept. The important characteristic of such systems is the neutron spectrum generated in the target under the action of the charged particle beam. Experimental data in this field are insufficient. The experiments with the big uranium target (BURAN) under preparation at the Laboratory of High Energies of the Joint Institute for Nuclear Research are aimed at filling this gap. The present numerical study addresses expected thermal, hydrodynamic and acoustic processes in this target and creates a background for the development of a novel acoustic method for energy loading diagnostics.

2. Problem setup and methods
2.1. Problem setup
The unique big uranium target BURAN (Fig. 1) has the following parameters: a length of 100 cm, a radius of 60 cm, the material is natural uranium. The target weight is $\sim 21$ tons. The cylindrical target has a through coaxial hole with a radius of 10 cm for replaceable converters made of different materials: nat$^3$U, Pb, Cu, Fe, Al, C. The converter is shorter than the target by 20 cm, leaving an air window at the front, so that the primary and secondary particles deposit most of their energy in the bulk of the target, rather than scatter backward. In the case of protons beam the energy was 660 MeV. In the case of deuteron (d), Li and C beams the energy was varied in the range from 300 to 2000 MeV/nucleon. With this combination of the target and beam parameters one can consider a quasi-infinite target. In other words, in this case the saturation of the energy deposition both in the longitudinal direction and along the radius is achieved [12]. The target from natural uranium of this size and mass, to our best knowledge, is unique, no analogs exist at research centers throughout the world. The capability to accelerate beams of protons and heavy ions up to gold with energies from 4 to 11 GeV/nucleon is unique for investigation of the secondary neutron spectrum, which is the key characteristic in the ADS concept. The problem is solved in two stages. At the first stage, the beam-target interaction is simulated via an open source code GEANT4 [13] to obtain the spatial distribution of the deposited energy. At the second stage, the calculated energy density flux field inside the target is used as the source for further thermal and hydrodynamic calculations.

Figure 1. Big uranium target “BURAN”.

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2.2. Model of accelerated particles interaction with matter

The code GEANT4 is used to simulate particle passage in the target, their interaction with matter, production of secondary particles and radiations. It was shown in [14] that GEANT4 reasonably well quantitatively describes the interaction of beams of intermediate energies (from hundreds of MeV to several GeV) with various targets from heavy materials with an accuracy of about 30%. The comparative analysis of numerical data obtained with GEANT4, MCNPX and SHIELD [15] also demonstrated satisfactory agreement between simulated and experimental data on ion beam interactions with thick targets on a level of accuracy about 30%. Experimental studies on the distribution of fissions inside an extended uranium target exposed to 0.5 – 4 GeV/nucleon deuteron beams [10, 16, 17] agree within 30% with GEANT4 simulations.

Figure 2a shows the integral energy deposition in the target for different beam energies ($E_{\text{dep}}$) as a function of the particle mass number ($A$).

![Figure 2a](image)

**Figure 2.** a) Energy deposited in the target as a function of the particle mass number for several beam energies. b) Relative contribution of the fission energy in the total energy released in the target as a function of kinetic energy per nucleon of incident ions for several ion species.

Low/intermediate energy (and highly charged) ions have short paths in the target, thus, the probability of inelastic interactions is low, and the power gain in the system drops. Uranium fission gives the main contribution to the power gain due to nuclear transformations. It was shown in [18] that the ratio of the fission cross section and the total cross section of inelastic interactions is $\sim 90\%$ for uranium and minor actinides and incident proton energies below 1 GeV, and this ratio decreases with increasing proton energy. Thus, for a known energy of one fission in uranium of 190 MeV, the relative contribution into the energy deposition in the target from fissions takes the form shown in Fig. 2b.

An important (and poorly experimentally studied) problem is the form of the spectrum of secondary neutrons produced in the bulk of the target. Therefore, the generation of secondary neutrons should be addressed with care. The well studied region of the neutron spectrum below 20 MeV was simulated via parameterizations based on the experimental data ENDF (Evaluated Nuclear Data File). Special attention was paid to simulation of inelastic hadronic interactions. For particles with energy above 50 MeV the Bertini cascade, Liege cascade, and binary cascade (BC) models were used to achieve the best agreement with experimental data obtained in experiments with bulk heavy targets. The total energy deposited in the target was obtained by summing all ionization losses, including ionization losses of $\delta$ electrons and gamma photon conversion, for all charged particles, both particles of the primary beam and all secondary particles from sequential nuclear reactions in the target: fission...
and multifragmentation fragments, produced and decaying charged particles till they are fully stopped or leave the target volume.

A converter from a light material (Li, Be) changes the shape of the neutron spectrum and increases the energy deposition in the target by a factor of 1.4–3; this effect is the strongest for light low-energy ions and targets from enriched uranium.

It should be noted that the use of standard sets of models (physics lists) of GEANT4 code and manual modifications to them may yield a discrepancy in the total energy deposition on a level of up to 50%, which makes experimental verification of existing models and codes quite topical problem.

3. Model of heat transfer

The problem of matter heating by an accelerated particle beam is as follows. An accelerated beam of proton, deuteron, Li, or C ions with an energy from 0.3 to 2.5 GeV/nucleon and an intensity of \(10^{10}–10^{11}\) particles per second hits the target and is stopped in it, depositing energy in the bulk of the target. Here, we consider the target heating by the beam, neglecting hydrodynamic effects in the heated target. In this case, according to the classical ideas [19], the energy balance in the target is written as follows:

\[
\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) + Q(\vec{r}, t),
\]

which is the heat conduction equation with a spatial thermal source. Here \(\rho\) is material density, \(c_p\) is heat capacity at constant pressure, \(T\) is temperature, \(\kappa\) is heat conductivity coefficient. The source is defined in a tabulated form of spatially distributed intensity (J/m\(^3\)) and a rectangular temporal pulse distribution,

\[
Q(\vec{r}, t) = Q(\vec{r}) \cdot \eta(t - t_0).
\]

The initial time instant was \(t_0 = 0\). The problem is axially symmetric, therefore, it is solved in the two-dimensional cylindrically symmetric formulation \((r, z)\):

\[
\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( \kappa \frac{\partial T}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial T}{\partial r} \right) + Q(\vec{r}, t).
\]

The expressions for the heat flux at the boundary of the target are:

\[q_z = -\kappa_{wall} \frac{\partial T}{\partial z} \bigg|_{wall},\]

\[q_r = -\kappa_{wall} \frac{\partial T}{\partial r} \bigg|_{wall}.\]

We assume that the external boundary of the uranium cylinder contacts with the ambient medium (air). Four variants of the boundary conditions are considered: (1) adiabatic wall \(q_z = 0, q_r = 0\), (2) isothermal wall with \(\kappa_{wall} = \kappa_U\), (3) isothermal wall with \(\kappa_{wall} = \kappa_{eff} = \frac{2\kappa_{air}\kappa_U}{\kappa_{air} + \kappa_U}\), (4) convective heat exchange with air. In the latter case, we perform an integrated calculation of thermal fluxes inside the target and in the air layer around the target. We also calculate convective flows in the air due to the target heating. The intensity of the process is rather low, therefore, the air around the target is heated slowly, and the resulting convective flows are characterized by low velocities. Thus, it is possible to apply the low compressibility approximation for the gas flow. In the low compressibility approximation, the total pressure \(p\) is represented as a sum of the background thermodynamic pressure \(\bar{p}(t)\) and the small perturbation \(\bar{p}(r, z, t)\), it is described by the following equations:

\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \bar{u}) = 0,
\]
\[
\frac{\partial \vec{u}}{\partial t} - \vec{u} \times \omega + \nabla H - \bar{p} \nabla (1/\rho) = \frac{1}{\rho} [\nabla \cdot \tau_{ij}], \tag{5}
\]
\[
\frac{\partial \rho h_s}{\partial t} + \nabla (\rho h_s \vec{u}) = D \bar{p} \frac{D}{Dt} + \nabla (\kappa_{\text{air}} \nabla T). \tag{6}
\]

Here, \(\rho\) is the air density, \(\vec{u}\) is the mass velocity of air, \(\omega \equiv \nabla \times \vec{u}\) is the vorticity, \(H \equiv |\vec{u}|^2/2 + \bar{p}/\rho\), \(\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right)\) is the viscous stress tensor, and \(h_s\) is enthalpy. The implicit difference scheme [20] is used for solution of the heat conduction equation in the target. The difference equation with an account of the boundary conditions and the given source term is solved by the alternating directions implicit integration method [21]. The predictor-corrector scheme described in detail in [22] is used for solution of the system of gas dynamics equations in the low compressibility approximation. The Poisson equation is solved via the classical successive over-relaxation method.

4. Hydrodynamic model

Acoustic oscillations are formed in the target as a result of the growing acoustic pressure at isochoric heating. This process is simulated by the system of hydrodynamic equations describing the propagation of low-amplitude perturbations in the target:

\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \vec{u}) = 0, \tag{7}
\]
\[
\frac{\partial \rho \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) (\rho \vec{u}) = -\nabla p, \tag{8}
\]
\[
\frac{\partial \rho E}{\partial t} + \nabla (\rho \vec{u} E) = -\nabla (\kappa \nabla T). \tag{9}
\]

Here, \(\rho\) is the medium density, \(\vec{u}\) is the mass velocity, \(p\) is the pressure, \(E = \varepsilon - |\vec{u}|^2/2\) is the total energy, \(\varepsilon\) is the internal energy, \(T\) is the temperature, and \(\kappa\) is the heat conduction of the medium.

The Mie-Gruneisen equations of state are applied to close the system of hydrodynamic equations:

\[
p = p_X + \Gamma \rho \varepsilon. \tag{10}
\]

The Birch–Murnaghan approximation of the cold curve is written as

\[
p_X = A \left( \delta^{1/3} - \delta^{-1/3} \right) \left[ 1 - B \left( 1 - \delta^{-2/3} \right) \right], \tag{11}
\]

where \(\delta = \rho/\rho_0\) is the relative compression. The amplitude of hydrodynamic oscillations in the target is small due to the low intensity of the process. Therefore, the cold curve is approximated by a linear function in the low-compression region:

\[
p_X - p_{X,0} = A (\delta - 1), \quad A = \rho c^2, \tag{12}
\]

where \(c\) is the speed of sound in the medium. The value of \(p_{X,0}\) is determined from the initial conditions. Equation of state in the following form is used for finding the temperature:

\[
d\varepsilon = c_p dT. \tag{13}
\]

The equation of state is obtained in the rigid body approximation in which \(c_p \approx c_V\).

In this study, the Gruneisen coefficients (\(\Gamma\)) for all metals was assumed to be equal to 2, and for graphite with a density of 1.8 g/cm\(^3\), \(\Gamma = 1\).
The boundary condition for the mass velocity and the pressure in the target is found from the following relations corresponding to the change of mass velocity and pressure at the boundary along the air Hugoniot curve and the release isentrope in a solid,

\[ P_1 - P_2 = -\rho U c (u_2 - u_1), \]  
\[ P_2 - P_0 = \rho_{air} c_{air} u_2. \]  

The unknown quantities and at the solid-air interface are determined as follows:

\[ P_2 = \frac{P_1 \rho_{air} c_{air} - P_0 \rho U c U _1 - u_1 \rho U c U}{\rho_{air} c_{air} - \rho U c U}, \]  
\[ u_2 = \frac{P_1 - P_0 - u_1 \rho U c U}{\rho_{air} c_{air} - \rho U c U}. \]  

5. Results and discussion

6. Transfer of the particle beam energy to the solid medium

Below we exemplify the deposited energy fields in the target (Fig. 3). The axial distribution of the deposited energy for different converter materials is shown in Fig. 4. The beam intensity is constant. Energy deposition is calculated according to the model presented in Section 2.2.

Figure 3. Distribution of energy deposited in the target by the 0.66 GeV proton beam: (a) U converter, (b) carbon converter. Color map is normalized to the maximum energy for each case. Lines show the numerical mesh; energy values are set at nodes.

7. Heat transfer inside the target

The kinetic energy of accelerated ions is converted into the internal energy of the target via elastic and inelastic nuclear interactions. The thermal energy spreads out from the beam absorption volume in the target via heat conduction. The heating of the target is limited by the heat flux from the target surface to the ambient medium. Let us first consider the regimes of target heating depending on the choice of the boundary conditions on the target surface. Since the target is surrounded by a relatively large volume of air at room temperature two asymptotic conditions can be applied on the target surface. The simplest case is the constant temperature of the target surface that is equal to the initial temperature 300 K. This is the isothermal approximation, herewith thermal evolution proceeds inside the target only. The opposite asymptotic is realized
Figure 4. Absorbed energy as a function of distance along the target axis for different target materials irradiated by the 0.66 GeV proton beam. Two thin vertical lines show the target boundaries along the $z$ axis.

Figure 5. Evolution of the average temperature of the target irradiated by 0.66 GeV proton beam calculated in three approximations: a) with adiabatic walls (blue line), with isothermal walls with effective heat transfer coefficient (green line) and with account of convective heat transfer in air (red line). b) with isothermal walls with effective heat transfer coefficient (green line) and isothermal walls with heat transfer coefficient of the target material (blue line).

if one takes into account that the thermal conductivity of air is much lower, as compared with a solid medium. In this case, the heat flux out from the boundary into the gas volume occurs to be much lower than the flux towards the boundary from the heated target. This case corresponds to the adiabatic boundary condition. In reality, both heat conductivity and heat capacity of the gas are much lower than those of the solid medium. Thus, the heat transfer in the gaseous medium is related not only to the molecular transport but also to the convection. Therefore, the solution should aim at the adiabatic asymptotic, the heat flux out from the target is assumed to be negligible.

Figures 5a and 5b illustrate the evolution of the average target temperature calculated for different boundary conditions. The solution with the account of heat conductivity in gas including gas convection is presented along with the solutions obtained in isothermal and adiabatic approximations in Fig. 5a. It can be seen that at the early stage all three solutions coincide with each other. At the later stage, the isothermal approximation determines
temperature saturation due to the equalization of the input energy by the heat flux from the solid medium to the environment at a constant temperature. At the same time, the adiabatic approximation defines the permanent heating of the target. As it was mentioned above the full model provides a solution close to the adiabatic one. Two isothermal approximations, namely with thermal conductivity on the wall surface $\kappa_{\text{wall}} = \kappa_U$ and $\kappa_{\text{wall}} = \kappa_{\text{eff}}$ are compared in Fig. 5b. It can be seen that for the case $\kappa_{\text{wall}} = \kappa_U$ the stationary temperature inside the target is achieved much faster ($\sim 3$ hours) than in the case $\kappa_{\text{wall}} = \kappa_{\text{eff}}$ ($\sim 400$ hours). The thermal conductivity of uranium $\kappa_U$ is much higher than the thermal conductivity in the air $\kappa_{\text{air}}$, thus the effective heat transfer $\kappa_{\text{eff}} \approx 2\kappa_{\text{air}}$, which is still much lower than $\kappa_U$. Such a difference between the heat transfer coefficients in the considered cases determines the higher heat flux out from the target surface in the case $\kappa_{\text{wall}} = \kappa_U$. Consequently, the higher heat flux results in the faster equilibration between energy deposition and energy outflow via heat transfer and achievement of a steady-state solution.

According to Fig. 5a, the effects of heat transfer in the gaseous medium become noticeable only on relatively long time intervals. Therefore, the convective transport via which the mass is flown away from the target surface (Fig. 6) and as a result the heat capacity of the adjacent gas layer decreases. Thus, the solution moves from the adiabatic asymptotic towards the isothermal one (Fig. 5a). Measuring the error $\delta = \frac{T - T_{\text{conv}}}{T_{\text{conv}} - 300} K$ between different approximations and calculations with account of convective heat transfer, one can estimate the time interval within which the error is less than 10%. Thus, isothermal approximation with $\kappa_{\text{wall}} = \kappa_U$ becomes inefficient at time instant $\approx 0.2$ h, isothermal approximation with $\kappa_{\text{wall}} = \kappa_{\text{eff}}$ is valid for $\approx 27.5$ h. For adiabatic approximation the error is less than 8% for the whole time period of observation.

It is important to note that the temperature field inside the target is spatially non-uniform (Fig. 7) and the maximal temperature corresponds to the Bragg peak of ion beam stopping, which depends on the converter material and the particle beam energy (Fig. 7).
Figure 7. Temperature profiles along the walls of the target irradiated by 0.66 GeV proton beam for different converters. a) Front end surface of the target, b) side surface of the target, c) rear end surface of the target.

Figure 8. Position of imaginary pressure gauges. (1) pressure gauge near the input window, (2) pressure gauge on the side wall of the converter, (3) pressure gauge on the rear end of the converter.

8. Acoustics generation
The permanent energy deposition into the medium induces the generation of the acoustic waves propagating in the whole volume of the target. Herewith, the acoustic wave (compression wave) pattern is determined by the deposited energy field. So, the compression wave is formed exactly in the region of energy absorption and then propagates in the bulk of the target.

To study the evolution of the pressure perturbations inside the target we record the amplitude of pressure oscillations at different points of the irradiated target (Fig. 8). At this, the magnitude of pressure perturbations is determined by the energy deposition intensity, while the frequency depends on the equation of state and the target geometry (Fig. 9). Figure 9 illustrates the pressure evolution inside the target near the air boundary for various converters and particle
energies. Figure 10 summarizes the data on the characteristic magnitudes and frequencies of the pressure signals. The perturbations generated by the energy deposition go to the ambient atmosphere as acoustic waves in the air. The characteristic frequencies of the acoustic waves lie in the audible range, however, the magnitudes in the considered cases are quite low. Nevertheless, such signals can be registered with sensitive pressure gauges that would open new possibilities for experimental diagnostic of the ion beam energy deposition, conversion and propagation in the bulk of the target.
Figure 10. Characteristics of the acoustic field for different converters irradiated by 0.66 GeV proton beam.

9. Conclusions
The developed physical and mathematical model and software codes provide direct modeling of the processes inside the target during long periods of irradiation (from a few microseconds to tens of hours). Four approximations of the heat exchange process between the target and the ambient atmosphere were considered. For time intervals of up to several hours all the approximations provide similar results. The most accurate solution is obtained via the convective heat exchange model and this approach is applicable during the longest time interval. The adiabatic approximation, however, gives results close to the convective approximation for a long time interval, and at the same time drastically reduces the calculation time. Despite the permanent irradiation, non-stationary periodic patterns of perturbations propagation are obtained for all converter materials. The perturbations amplitude depends on the irradiation intensity and implemented equation of state of the converter material. Thus, the highest acoustic perturbation amplitude is observed at the gauge located on the front surface of the irradiated material for the uranium converter. Accurate analysis of the amplitude-frequency characteristics requires more detailed research. The obtained results on the acoustic perturbations generated in the bulk target irradiated by an accelerated particle beam give grounds for development of a novel experimental measurement technique based on pressure sensors to characterize the inner state of a bulk target loaded by an ion beam.

The model is well suited for investigation of the physical basics of accelerator-driven system and proof-of-principle for accelerator-driven systems, the topic included in the research program of the NICA collider of the Joint Institute for Nuclear Research accelerator complex. It will be used for theoretical predictions of experimental conditions of bulk target irradiation to assist experiment setting, for verification of existing physical models and computer codes (in combination with experiment), and for the study and optimization of the accelerator-driven system target parameters.
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