Modelling of desublimation of large cryogenic pellets for the ITER Shattered Pellet Injector

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The disruption mitigation concept of ITER is based on the injection of small fragments originating from large cryogenic pellets made of hydrogen, neon or mixtures thereof[1]. The foreseen pellets are up to 28.5 mm diameter and 57 mm long cylinders. These are planned to be desublimated in a barrel, accelerated up to 600-800 m/s velocity with a high pressure gas impulse, broken into small pieces on a shatter plate, and enter the plasma as a spray of small pellet fragments[2], known as Shatter Pellet Injection (SPI).

Such large pellets have not been used on present-day devices. In particular, formation of large hydrogen pellets will be challenging due to their low triple point temperature and heat conduction. In order to develop the ITER-relevant SPI technology a Support Laboratory for the Disruption Mitigation System is being set up at the Centre for Energy Research, Budapest, Hungary in the framework of an ITER contract. This paper presents the *PFreeze* code and some of its results which intend to study the desublimation process of these large pellets.

The model

The model assumes axial symmetry around the barrel centreline and mirror symmetry around the plane perpendicular to the cold head centre as shown in *Fig. 1*. Cylindrical *r,z* coordinate system is used. The actual pellet surface as a function of time is described by the $r_i(z,t)$ function which imposes some limitation on the pellet shape. The Q_r and Q_z (radial, axial) heat fluxes and the resulting temperature change are calculated in the pellet material and the barrel wall using standard heat diffusion equations:

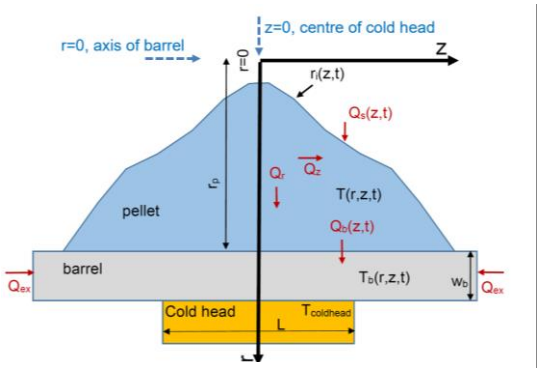

Fig. 1. Modelling geometry.

$$Q_r(r,z,t) = -\kappa \frac{\partial T(r,z,t)}{\partial r}, \qquad Q_z(r,z,t) = -\kappa \frac{\partial T(r,z,t)}{\partial z}, \tag{1}$$

$$c\rho \frac{\partial T(r,z,t)}{\partial t} = -\left[\frac{1}{r}\frac{\partial \left(rQ(r,z,t)\right)}{\partial r} + \frac{\partial \left(Q(r,z,t)\right)}{\partial z}\right]. \tag{2}$$

The temperature dependent κ,c,ρ material constants (heat diffusivity, specific heat and density, respectively) were taken from an extensive literature survey. The temperature of the cold head

and the axial heat flux along the barrel wall are taken as fixed parameters. The p gas pressure and T temperature inside the barrel is assumed to be uniform far from the pellet and barrel surface.

Desublimation and surface heat flux

The heat flux on the pellet and barrel surface and the desublimation flux is calculated self-consistently from first principles using two parameters; the α_s sticking coefficient giving the probability that a gas molecule hitting the pellet or wall surface sticks to it, and the α_E energy accommodation coefficient describing the energy change of a gas molecule reflected from the T_S temperature surface:

$$\alpha_E = \frac{E_r - E_{in}}{E_s - E_{in}}, \qquad E_{in} = \gamma k T, \qquad E_s = \gamma k T_s. \tag{3}$$

Currently α_s=0.8, α_E=0.8 (pellet) and α_E=0.5 (barrel) is used. The Φ_S desublimation flux is calculated from the experimentally known $p_{sat}(T)$ saturation pressure by balancing the sublimation and desublimation processes:

$$\Phi_s(p,T,T_s) = \frac{1}{\sqrt{2\pi k m}}\left[\alpha_s(T)\frac{p}{\sqrt{T}} - \alpha_s(T_s)\frac{p_{sat}(T_s)}{\sqrt{T_s}}\right]. \tag{4}$$

The heat flux heating the pellet surface is composed of the desublimation energy H_s, the energy difference between molecules in the gas and the solid phase and the heating by reflected molecules:

$$Q_s^{pellet}(p,T,T_s) = \frac{1}{\sqrt{2\pi k m}} H_s\left(\alpha_s(T)\frac{p}{\sqrt{T}} - \alpha_s(T_s)\frac{p_{sat}(T_s)}{\sqrt{T_s}}\right) + \frac{p\,\gamma k(T - T_s)}{\sqrt{2\pi k T m}}[\alpha_s(T) + (1-\alpha_s)\alpha_E]. \tag{5}$$

The heat flux out from the gas does not contain the desublimation energy but it contains the cooling effect of the molecules sublimated from the surface into the gas:

$$Q_s^{gas}(p,T,T_s) = \frac{1}{\sqrt{2\pi k m}}\gamma k(T - T_s)\left[\frac{p}{\sqrt{T}}(1-\alpha_s)\alpha_E + \alpha_s(T_s)\frac{p_{sat}(T_s)}{\sqrt{T_s}}\right] \tag{6}$$

For Eqs. (4)-(6) the temperature of the gas at the surface would be needed which, in general, would necessitate a 2D gas flow modelling in the barrel. To simplify, we assume one-directional gas flow perpendicular to the solid surface and write the equation of the gas temperature distribution $T'(y,t)$ in the following form:

$$\frac{\partial T'}{\partial t} = \frac{\kappa_{gas}}{\rho_{gas} c_p}\frac{\partial^2 T'}{\partial y^2} - v\frac{\partial T'}{\partial y}, \tag{7}$$

where y is the coordinate perpendicular to the surface and v is the gas velocity. Expressing the velocity from the desublimation flux, the gas density from the pressure and temperature and assuming that κ_{gas}/c_p is constant the steady-state solution of Eq. (5) can be calculated:

$$T'(y) = (T - T_0)e^{-y/L_T} + T_0, \qquad L_T = \frac{\kappa_{\mathrm{gas}}}{\Phi_s \gamma k}, \tag{8}$$

where T_0 is the fixed gas temperature far from the surface. If the L_T scale length is considerably smaller than the free barrel diameter this approximation is valid. The numerical model shows that this is almost always the case. From Eq. (8) the heat flux in the bulk gas can be calculated as $Q_s^{gas} = \Phi_s \gamma k T_0$ which, in steady-state, should be equal to Eq. (6). The numerical solution of this by taking the desublimation flux from Eq. (4) yields the self-consistent surface gas temperature and the desublimation flux.

Numerical scheme

In the axial direction a fixed equidistant z mesh is used both in the pellet and the barrel. In the radial direction coordinate r is replaced by a new coordinate $x(r,z)$ moving with the changing pellet layer thickness: $x(r_p)=0$ and $x(r_i,z)=1$. The heat diffusion equations are rewritten for the x,z coordinates using the appropriate partial derivatives of the $x(r,z)$ and $r(x,z)$ functions. Where the barrel is free from desublimated pellet material ($r_i(z)=r_p$) this coordinate transformation is not possible. Therefore, for z coordinates where the pellet material thickness is less than 0.5 mm the heat diffusion equation is not solved in the pellet, but the barrel surface temperature is used for the pellet material.

The pellet surface $r_i(z)$ time evolution is calculated by moving the r_i points perpendicular to the local pellet surface by $\Phi_s dt\, m/\rho$ distance, where dt is the time step. The resulting curve is interpolated to the z-mesh. As the pellet grows in a minute-hour time scale dt is chosen to be 0.1-1s. With this time step the heat diffusion equation cannot be solved, it needs a time step in the μs time scale. Therefore, the heat diffusion is solved with a small time step until approximately steady state is reached then the pellet shape is stepped. This way the calculation time is reduced to about 50-100 hours on a single CPU using a the Python language code.

The calculation is stopped when a given pellet Aspect ratio is reached: $A = L_{min}/L_{max}$, where the two lengths are the minimum and maximum length of the pellet in the barrel.

Results

Modelling runs were done for H,D and Ne pellets and 19, 28.5 mm barrel inner radius and $L=4r_p$. It was found that, to limit the pellet length to the cold head length, Q_{ex} should reach a certain value (about 0.8 W for r_p=28.5mm, w_b=2.6mm) so as the temperature gradient is sufficiently steep at the end of the cold head. The barrel pressure should be below 50 mbar, otherwise the too strong pellet surface warming raises the temperature above the triple point. A typical result is shown in *Fig. 2*. The temperature and heat flux distribution at t=500 s is in the left column, the time evolution of certain parameters are in the rightmost column. One can see that reaching A=0.9 needs about the same time as closing the hole in the middle of the pellet. The gas flow rate changes about 2 orders of magnitude during the process and the power to the

cold head and the gas precooler is ~5W in the first 100s. There is a significant temperature gradient across both the barrel wall and the pellet as shown in the middle-bottom plot.

Conclusions

The PFreeze code indicates that creating 28.5 mm diameter D/H pellets with 5K cold head temperature takes about 40/50 minutes. If the cold head temperature is 8K the process takes even longer, 60/90 minutes. This is in rough agreement with experimental findings[3]. Preparation time is set by the heat propagation through the pellet material which slows down the desublimation process as the pellet layer becomes thicker.

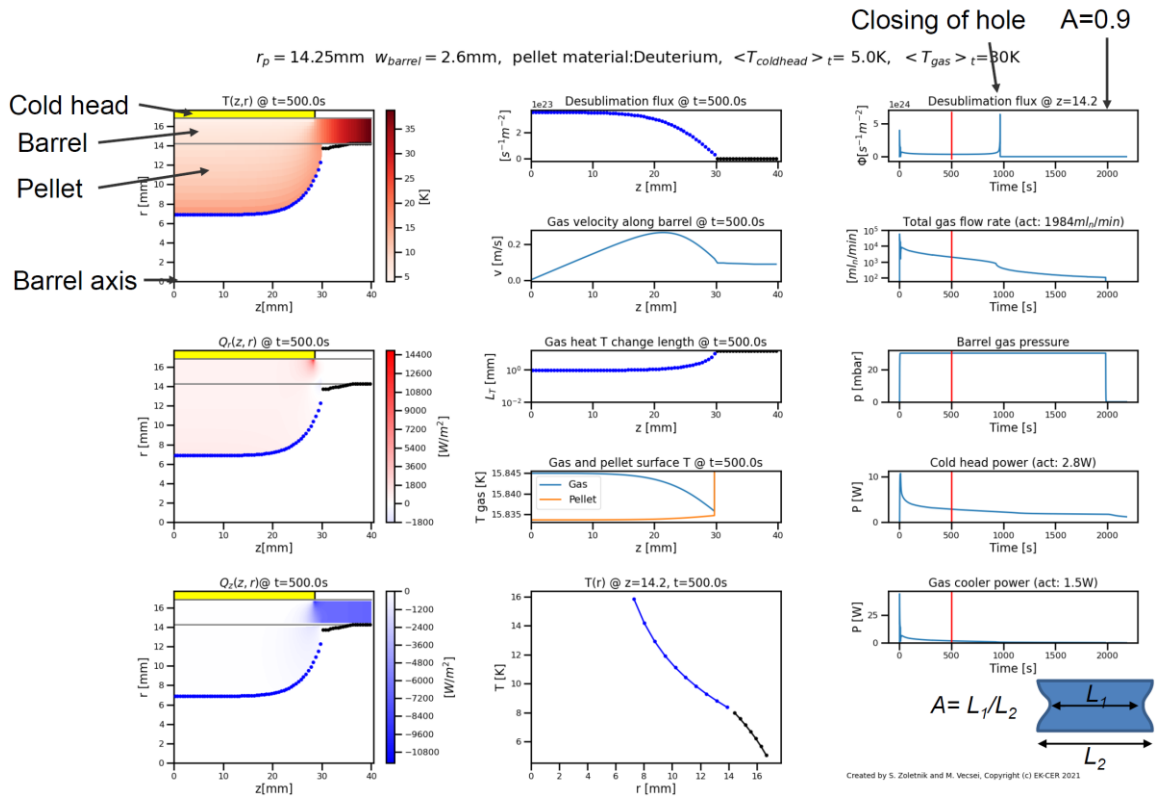

Fig. 2. Result of a Deuterium pellet calculation.

The work has been performed as part of the ITER DMS Task Force programme. The DMS Support Laboratory has received funding from the ITER Organization. The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.

References

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