JOURNAL OF RESEARCH of the National Bureau of Standards—C. Engineering and Instrumentation
Vol. 65C, No. 2, April–June 1961

Analog Simulation of Zone Melting

H. L. Mason

(January 13, 1961)

An analog computer was used to simulate zone melting in small-diameter tungsten rods of 0.2 to 1 centimeter. Heat balance equations take account of electron bombardment, heat capacity, radial conduction, axial conduction, and surface radiation. Diagrams are given for the chosen spatial subdivision and for the computer mechanization. Predicted temperature-time curves are shown for a rod of 0.4-centimeter diameter with optimum power input of 650 watts. Unsatisfactory operation is predicted for zone melting of a 1-centimeter rod.

As part of the NBS program for attempting to supply metal samples so pure that no spurious lines can be detected by spectroscopy, G. A. Moore of the Chemical Metallurgy Section has developed an apparatus for zone melting of small-diameter tungsten rods. Because of the high cost of the semi-purified material used in the process, it became desirable to simulate the heat transfer operation as a means of determining optimum relations between rod diameter, heating rate, and progress of the molten zone.

The technique is applicable to other materials, and the problem is interesting from the simulation viewpoint for several reasons. The conventional diffusion equation frequently used for analog computation is not suitable because it requires precise knowledge of the temperature distribution at the surface. A model must be set up in terms of heat flows; these too are unknown, but can more readily be estimated from the physical situation. The model must include radiation losses, which at these high temperatures require fourth-power nonlinear terms. The change of state at the melting point results in a local interruption of the temperature rise in the melting zone. Conductivity, thermal capacity, and emissivity will change with temperature and with state. Time rates of temperature change will be treated as infinitesimals, spatial rates as discrete increments. The incremental dimensions for radial and axial subdivision must be carefully chosen if optimum use is to be made of the limited number of integrating amplifiers available.

The radii r_s of the 5 rods to be simulated range from 0.1 to 0.5 cm; lengths (actually 3 or 4 ft) are assumed infinite. Heating is by continuous electron bombardment in a vacuum from a heated wire of 1.2 mm diameter, shaped to an annulus of 4.0-cm diameter surrounding the rod as shown in figure 1. The heater is initially fixed near one end, but after melting begins it is moved very slowly up (or down) the rod. The impurities are retained in the molten zone and are carried to one end, leaving the purer metal to solidify again to rod form. This motion is neglected in the simulation. Circumferential symmetry and an isomorphic rod are assumed, and the heat input from the wire is taken to be a step function of time.

Because of symmetry on either side of the heater midplane, it is enough to consider only half the length of the rod. Preliminary estimates indicated that temperatures would rise only slightly at points 20 mm distant from that plane, so that heat flow beyond this was neglected. Steep temperature gradients may be expected near the heater, and it is necessary to assure that metal will not drip off the outer surface before the core is melted. One purpose of the simulation, therefore, was to find whether the molten zone advanced radially at least as fast as it advanced axially. Subdivisions into annuli or cylinders with lengths Δy, outer radii r_o, and inner radii r_i were decided upon. Their generalized proportions relative to surface radii r_s are given in table 1.

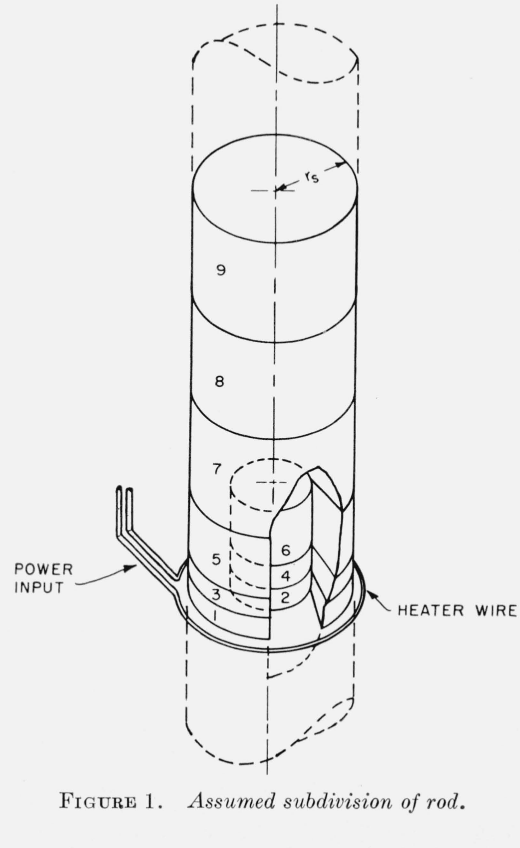

FIGURE 1. *Assumed subdivision of rod.*

The heat stored per unit time in zone 1, which is assumed to have a uniform temperature of T_1 degrees Kelvin, at time θ seconds after heating begins, is the thermal capacity of the zone volume multiplied by the rate of temperature rise. With density γg/cm^3 and temperature-dependent specific heat $c=c(T_1)$ cal/g-deg K, this storage rate is $\gamma c\pi(r_s^2-r_i^2)\Delta y\, dT_1/d\theta$. Similar expressions hold for the other zones, with r_o replacing r_s and $r_i=0$ for the inner ones.

TABLE 1.

Zone	r_o/r_s	r_i/r_s	Δy
			Mm
1	1	0.5	1
2	0.5	0	1
3	1	0.5	1
4	0.5	0	1
5	1	0.5	3
6	0.5	0	3
7	1	0	5
8	1	0	5
9	1	0	5

Heat inflow to zone 1 will be 239 P cal/sec, where P is the steady kilowatt power input to the half-rod. Heat outflow by reason of conductivity $k=k(T_1)$ cal/(sec) (cm)^2 (deg K/cm) will be radially inward to zone 2 across the area $2\pi r_i\Delta y$ with the gradient $(T_1-T_2)/(r_1-r_2)$, where r_1 and r_2 are mean radii. Also, there will be conduction axially to zone 3, at the rate $\pi k(r_s^2-r_i^2)\ (T_1-T_3)/(y_1-y_3)$ where y_1 and y_3 are mean lengths. No heat is transferred beyond the heater midplane, since there is no gradient across that boundary. However, zone 1 loses heat by radiation to ambient temperature T_a at the rate $1.37\epsilon\,(2\pi r_s\Delta y)\,[(T_1/1000)^4-(T_a/1000)^4]$ where $\epsilon=\epsilon(T_1)$ is the temperature-dependent emissivity. The heat flow balance equation for zone 1, at any time up to the instant of local melting, is then

$$\gamma c\pi(r_s^2-r_i^2)\Delta y\,\frac{dT_1}{d\theta}=239P-2\pi r_i k\Delta y\left[\frac{T_1-T_2}{r_1-r_2}\right]$$

$$-\pi k(r_0^2-r_i^2)\left[\frac{T_1-T_3}{y_1-y_3}\right]$$

$$-1.37\epsilon(2\pi r_s\Delta y)\left[\left(\frac{T_1}{1000}\right)^4-\left(\frac{T_a}{1000}\right)^4\right].$$

Similar heat flow balance equations can be written for the other zones except that $239P$ is replaced by radial or axial conductive inputs, and there is no radiation for the interior zones where r_0 replaces r_s and $r_i=0$.

For zone 3, for example, the equation is

$$\gamma c\pi(r_s^2-r_i^2)\Delta y\,\frac{dT_3}{d\theta}=-2\pi r_i k\Delta y\left[\frac{T_3-T_4}{r_3-r_4}\right]$$

$$+\pi k(r_s^2-r_i^2)\left[\frac{T_1-T_3}{y_1-y_3}\right]-\pi k(r_s^2-r_i^2)\left[\frac{T_3-T_4}{y_3-y_4}\right]$$

$$-1.37\epsilon(2\pi r_s\Delta y)\left[\left(\frac{T_3}{1000}\right)^4-\left(\frac{T_a}{1000}\right)^4\right]$$

Numerical values of the properties γ, c, k, and ϵ were known only imprecisely for tungsten, but it appeared that they change only slowly in the range from $T_a=300$ to $T_m=3700$, the melting point. Accordingly, the values of table 2 were used in the computation, based on preliminary estimates of temperatures with zone 1 melted and zones 2 and 3 just beginning to melt. The heat of fusion in zone 1, about 44 cal/g, was neglected in this approximation. For each zone, the initial temperature was assumed to be 300 °K, and regions beyond zone 9 were assumed to remain at this temperature.

Substitution of numerical values in the 9 expressions for heat flow gave for the rod of 1-cm diameter the following set of simultaneous first-order difference-differential equations for solution by the analog computer:

$$+0.2\dot{T}_1=.015\mathrm{P}-.0394(T_1-T_2)-.369(T_1-T_3)$$
$$-.0498\mathrm{T}_1^4/10^6$$
$$-2\dot{T}_2=-.118(T_1-T_2)+.363(T_2-T_4)$$
$$-0.2\dot{T}_3=-.369(T_1-T_3)+.0388(T_3-T_4)+.173(T_3-T_5)$$
$$+.0498T_3^4/10^6$$
$$+0.2\dot{T}_4=+.406(T_2-T_4)+.1302(T_3-T_4)-.23(T_4-T_6)$$
$$+0.2\dot{T}_5=+.439(T_3-T_5)-.3195(T_5-T_6)-.261(T_5-T_7)$$
$$-.134T_5^4/10^6$$
$$-2\dot{T}_6=-.115(T_4-T_6)-.2116(T_5-T_6)+.067(T_6-T_7)$$
$$-\dot{T}_7=-.129(T_5-T_7)-.0504(T_6-T_7)+.167(T_7-T_8)$$
$$-\dot{T}=-.167(T_7-T_8)+.167(T_8-T_9)$$
$$+\dot{T}_9=+.167(T_8-T_9)-.167T_9+.502$$

TABLE 2

Zone	T	γc	k	ϵ
1	3700	0.84	0.31	0.36
2	3700	.84	.31	----
3	3700	.84	.31	.36
4	3000	.75	.30	----
5	1100	.55	.27	.13
6	700	.50	.39	----
7, 8, 9	500	.50	.42	.05

Figure 2 shows the computer patchboard diagram for the first two and last two of these equations. The time scale was slowed in the ratio of 1:20, and 1 machine volt represented 100° Kelvin. Heater input P was adjusted by trial with the aim of establishing an optimum value which would use a minimum of energy without causing zone 3 to melt ahead of zone 2. For the 1-cm rod, such a value could not be found, since zone 3 always reached 3,700° before zone 2, while the temperature of zone 1 went up to about 4,600°. This represents an undesirable physical situation which in practice may prevent satisfactory processing of a rod of this large diameter. In view of the uncertainty as to actual values of γ, c, k, and ϵ, it was considered unnecessary to carry through the computation for a more refined approximation.

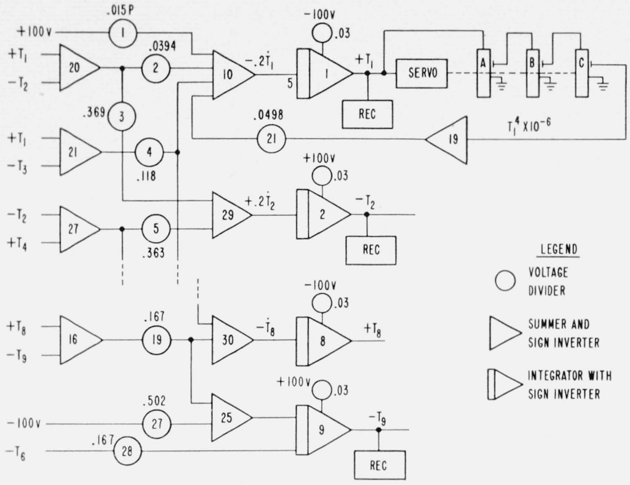

FIGURE 2. *Initial and final stages of computer patching.*

A set of temperature-time curves for one of the smaller rods with a 650-watt input is shown in figure 3. It will be noted that the melting of zone 3 lags that of zones 1 and 2, and hence that the power can be adjusted so that zone 3 just fails to melt. This assures formation of a thin liquid layer which is physically stable. The rod is nearly melted through in about 3 sec. This finding required modification of the power control circuits of the experimental apparatus by addition of rapid-response components to supplement the original servomechanism, which had required about 30 sec to establish an equilibrium setting.

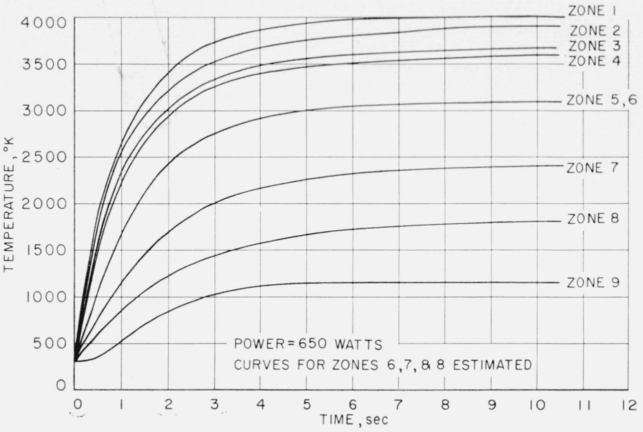

FIGURE 3. *Zone melting 2-mm-radius tungsten rod.*

Assistance on this problem came from NBS colleagues G. A. Moore, who supplied the physical constants and offered much constructive advice; P. K. Wong, who operated the computer; and R. Shives, who plotted the curves.

(Paper 65C2–60)