Field Precision LLC

KB

Simulation Suite for Shock Hydrodynamics and Detonations

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Contents

1 Introduction – installation and activation

KB is a suite of 1D/2D computer programs and data resources to model matter at extreme pressures and temperature. The primary application is simulation of shocks and detonations. The finite-element Lagrangian methods applied are applicable to self-connected assemblies that undergo extreme changes in pressure and temperature. They are not intended for calculations of collisions between separated objects or other problems involving transitory voids. The programs run under 64-bit versions of Windows.

To install the **KB** package, download and run the executable `kbinstall.exe`. The automatic installer creates the directory

```
c:\fieldp\kb
```

and organizes programs and documents within the directory. The installer also adds a **KB** icon to your desktop and a program group to your start menu to run the **KB** program launcher. The main technical programs will not function until you activate the software. Follow the instructions sent with the download information. To get started, click the Activate button in the program launcher. To remove the package, you can use either the deinstaller in the start menu group or the standard Windows procedure. The locations and functions of the package components are listed in Table 1.

It is good practice to keep your data separate from the program directory. Create a working directory and then subdirectories to store different types of calculations. We shall call the current directory the *data directory*. To set up a **KB1** or **KB2** calculation, you need to move all required resources to the data directory. For a **KB2** calculation, resources may include the following file types:

`RUNAME.MIN`, definition of the 2D geometry, input to **Mesh**.

`RUNNAME.KIN`, run control script, input to **KB2**.

`MATNAME.KBT`, **KB** tables that will be referenced.

`WAVEFORM.PRS`, pressure waveforms and other tabular data.

All output files will be written to the data directory.

The most convenient way to carry out a run is to use the **KB** program launcher. Click on the desktop icon to display the dialog of Fig. 1. The *Program directory* is the location where **KB** looks for executable programs and this manual. The default is `c:\fieldp\kb`. The first step is to define the data directory. Use the *Set data directory* command to move to the location where you put the input files. **KB** records the directory sets it the the next time it runs.

From this point, program operation is simple. Click the button next to the program you want to run. After loading, the selected program will be ready to seek input files from the assigned data directory. You can change the data directory at any time. If a program is missing, nothing will happen when you press the corresponding button. The analysis programs `kb1v.exe`, `kb2v.exe` and `probe.exe` will seek output files in the current data directory.

Table 1: Components of the **KB** package

Directory	**File**	**Function**
\kb	kb.exe	Utility to launch **KB** programs
\kb	kb1.exe	1D hydrodynamic solutions
\kb	kb1v.exe	Spatial data analysis, **KB1**
\kb	probe.exe	Temporal data analysis
\kb	mesh.exe	2D mesh generator for **KB2**
\kb	kb2.exe	2D hydrodynamic solutions
\kb	kb2v.exe	Spatial data analysis, **KB2**
\kb	kbview.exe	Utility for hydrodynamic calculations using the **KB** tables
\kb\kbtable	name.kbt	Equation-of-state data table at high pressure and temperature for 141 materials
\kb\resources	shockeos.txt	Shock equation-of-state parameters for 417 materials
\kb\resources	explode.txt	Denotation parameters for 29 materials
\kb\resources	hugocalc.xls	Spreadsheet to calculate Hugoniot curves from shock EOS parameters
\kb\kb1examp		Ready-to-run input files for **KB1**
\kb\kb2examp		Ready-to-run input files for **KB2**

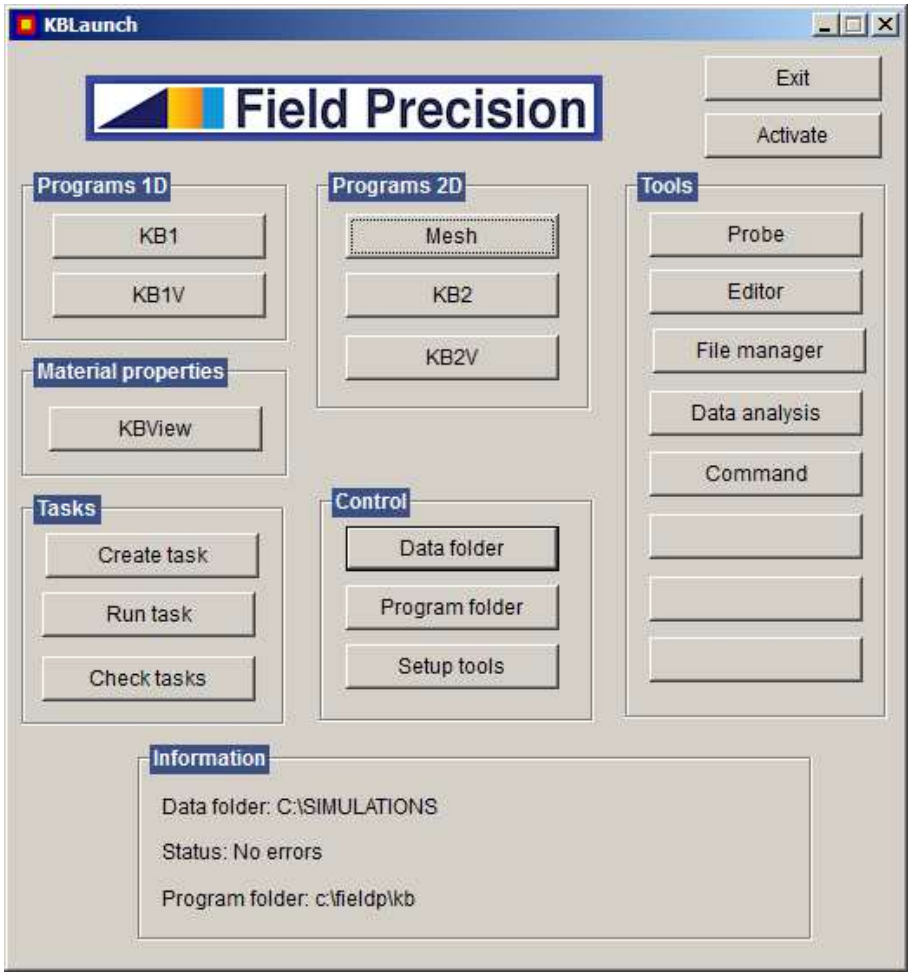

Figure 1: **KB** program launcher

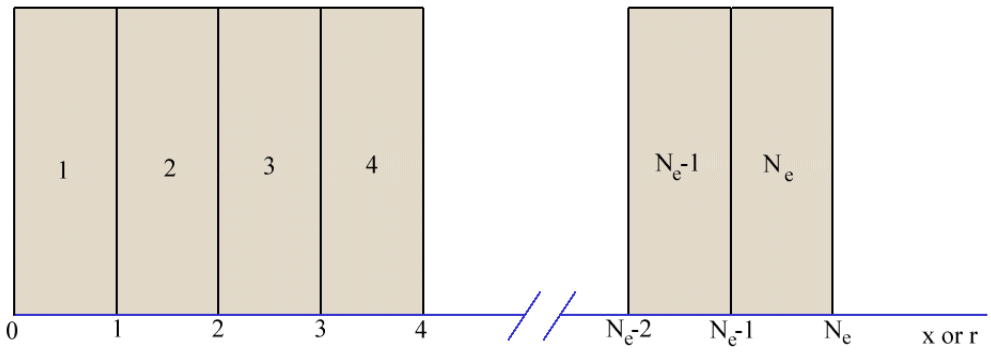

Figure 2: Index conventions used in **KB1**.

2 Physics of the KB codes

2.1 One-dimensional equations of hydrodynamics

The hydrodynamic equations used in **KB1** are difference representations of conservation of mass, momentum and energy applied over elements[1]. Figure 2 shows element divisions for a one-dimensional simulation. Depending on symmetry, the slices represent thin plates, cylindrical shells, or spherical shells. The two sets of indices shown apply to elements and element boundaries (*nodes*). Boundary quantities are denoted with upper case letters and element quantities with lower case. For example, Element i with average radius r_i has boundaries at R_{i-1} and R_i. Elements retain their material identity as they move and change size during the calculation. The method is similar to Lagrangian finite-difference calculations[2]. The approach is not suited for modeling processes like mixing and collisions of initially separated objects. On the other hand, the element-centered approach has two advantages:

Automatic zone refinement for compressional phenomena like shocks.

Ability to model explosive processes where the solution volume size may change by orders of magnitude.

In this discussion we shall concentrate on cylindrical systems. The extension to planar and spherical systems is straightforward. Conservation of mass implies that element masses do not change during the simulation. Consider an element with initial boundaries R_{0i-1} and R_{0i} and initial density ρ_{0i}. The mass is given by

$$m_i = \rho_{oi}\pi(R_{oi}^2 - R_{oi-1}^2). \tag{1}$$

The boundaries move in response to forces. The density at any time is related to the boundary positions by

$$\rho_i = \frac{m_i}{\pi(R_i^2 - R_{i-1}^2)}. \tag{2}$$

Note that Eqs. 1 and 2 do not employ approximations based on small element width. This feature avoids numerical problems when elements compress to cylindrical or spherical axes.

Furthermore, the model allows the use of large elements. The average element radius corresponds to the center-of-mass coordinate. Assuming a uniform density, the average radius of a cylindrical element is related to the boundary radii by

$$r_i = \sqrt{\frac{R_i^2 + R_{i-1}^2}{2}}. \tag{3}$$

We express conservation of momentum as an equation of motion for element boundaries. The object is to find the boundary velocities

$$V_i = \frac{dR_i}{dt}. \tag{4}$$

The time rate-of-change of momentum at boundary i equals the time derivative of velocity times half the masses of adjacent elements,

$$\left(\frac{m_{i+1} + m_i}{2}\right) \frac{dV_i}{dt}. \tag{5}$$

The force on the boundary is the sum of forces from adjacent elements. Summing pressure forces gives the equation of motion

$$\left(\frac{m_{i+1} + m_i}{2}\right) \frac{dV_i}{dt} = (-p_{i+1} - w_{i+1} + p_i + w_i)2\pi R_i. \tag{6}$$

The new element quantities introduced in Eq. 6 are the pressure p_i and the artificial viscosity force w_i. The pressure force equals the difference in pressure in the adjacent elements multiplied by the cylindrical area at the boundary. The artificial viscosity force term damps non-physical oscillations at shock fronts. The physical rationale for artificial viscosity and its inclusion in the hydrodynamic equations are covered in Ref. [2]. **KB1** employs an adaptation of the von Neumann-Richtmeyer form[3, 4] used in finite-difference solutions,

$$w = -C\rho\Delta^2 \left|\frac{\partial v}{\partial x}\right| \frac{\partial v}{\partial x}. \tag{7}$$

The quantity C in Eq. 7 is an adjustable parameter with value near unity to spread the shock over several elements, Δ is the element scale length, and ∂v/∂x is the spatial derivative of velocity. **KB1** employs the following difference representation for Eq. 7:

$$w_i^n = -C\rho_i^n |V_i^{n-\frac{1}{2}} - V_{i-1}^{n-\frac{1}{2}}| (V_i^{n-\frac{1}{2}} - V_{i-1}^{n-\frac{1}{2}}). \tag{8}$$

KB1 advances hydrodynamic quantities using the time-centered leap-frog method[2]. The boundary velocities V_i are defined at half time steps and all other quantities apply at integral steps. Throughout this discussion the superscript n denotes the time step, so that $t^{n+1/2} = t^n + \Delta t/2$. Replacing time derivatives in Eq. 6 with time-centered difference operators gives an equation to advance the boundary velocity,

$$V_i^{n+\frac{1}{2}} = V_i^{n-\frac{1}{2}} - \left(\frac{\Delta t}{m_{i+1} + m_i}\right) \left[(p_{i+1}^n + w_{i+1}^n - p_i^n - w_i^n)4\pi R_i^n\right]. \tag{9}$$

Given the modified velocities, the next step is to advance the boundary radii to the next integral time step,

$$R_i^{n+1} = R_i^n + V_i^{n+\frac{1}{2}} \Delta t. \tag{10}$$

New element densities and average radii can be determined from $R_i^{n+1/2}$ using Eq. 2.

The internal energy U_i is an element property equal to the material energy of element i divided by m_i. **KB1** does not model changes of U_i resulting from radiation transport. Electron thermal conduction contributions are also neglected for three reasons:

> Thermal conduction in solids and liquids is negligible compared to energy transport by shocks.
>
> Thermal transport coefficients are not well known at high temperature and pressure.
>
> Energy transport in gases and plasmas is usually dominated by convection.

Under the limiting assumptions, changes of internal energy in hydrodynamic calculations result from work performed by pressure, the artificial viscosity force and elastic stress. The work performed by pressure and artificial viscosity force on element i in a time step is $-(p_i + w_i)\Delta V_i$, where ΔV_i is the change in element volume. The equation to advance internal energy is

$$U_i^{n+1} = U_i^n + \frac{1}{m_i}\left[-\frac{(p_i^{n+1} + p_i^n)}{2}\pi({R_i^{n+1}}^2 - {R_i^n}^2 - {R_{i-1}^{n+1}}^2 + {R_{i-1}^n}^2)\right]. \tag{11}$$

The first term in brackets is a time-centered expression involving the advanced value of pressure. The advanced pressure is estimated by the two-step process described in the next paragraph.

To close the set of equations we must find the new element pressures p_i^{n+1} corresponding to modified values of density and internal energy, ρ_i^{n+1} and U_i^{n+1}. The values are determined from the equation-of-state relationships discussed in Chaps. 3 and 4. The **KB** tables contain values of pressure and internal energy as functions of density ρ and temperature τ: p(ρ,τ) and U(ρ,τ). With known values of density and internal energy the temperature τ can be determined through an inverse interpolation. **KB1** uses a modified two-step method[2] to advance the pressure and to preserve time-centering in Eq. 11. The advanced internal energy U_i^{n+1} is first estimated from Eq. 11 using only p_i^n. Equation-of-state relations give estimates of the advanced pressure p_i^{n+1}. The quantity $(p_i^n + p_i^{n+1})/2$ is then substituted in Eq. 11 to yield an improved value U_i^{n+1}. Equation-of-state interpolations are repeated at the new pressure p_i^{n+1} and (for materials represented by **KB** tables) the new temperature τ_i^{n+1}.

2.2 Shock equations

The differential equations for conservation of mass and momentum at a point in a fluid are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{12}$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) = -\nabla p. \tag{13}$$

The quantities in Eqs. 12 and 13 are the density ρ, velocity v, and pressure p. For a one-dimensional disturbance in the limit of small velocity, the linearized equations are

Table 2: Hydrodynamic quantities in **KB1**

Symbol	**Description**	**Units**
r	Average element position	m
R	Element boundary position	m
m	Element mass	kg
V	Element boundary velocity	m/s
Δt	Time step	s
p	Pressure	Pa (newtons/m^2)
w	Artificial viscosity	Pa (newtons/m^2)
U	Internal energy	J/kg

$$\frac{\partial \rho}{\partial t} = -\rho \frac{\partial v}{\partial x}, \tag{14}$$

$$\rho \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x} = -\frac{\partial p}{\partial \rho}\frac{\partial \rho}{\partial x}. \tag{15}$$

The derivative $\partial p/\partial \rho$ is a characteristic of the medium, independent of position and time. Therefore, Eqs. 14 and 15 imply that

$$\frac{\partial^2 \rho}{\partial t^2} = \left(\frac{\partial p}{\partial \rho}\right)\frac{\partial^2 \rho}{\partial x^2}. \tag{16}$$

Equation 16 describes small amplitude compression waves that move through the medium at the sound speed

$$C_s = \sqrt{\frac{\partial p}{\partial \rho}}. \tag{17}$$

Given an equation of state for the material, we can determine how C_s varies with pressure and density. As an example, consider a γ-law ideal gas[5]:

$$p = A\rho^\gamma. \tag{18}$$

Equation 18 implies that the change of pressure with density is

$$\frac{\partial p}{\partial \rho} = C_s^2 = A\gamma\rho^{\gamma-1}, \tag{19}$$

In a perfect gas with $\gamma = 1$, the compressibility (and hence the sound speed) is independent of density. Real gases (and most solid and liquid materials) become less compressible at high density because of overlap of electron shells. In this case, γ is greater than unity and hence the sound speed increases with density and pressure. This fact accounts for the existence of shocks.

A *shock* is a sharp discontinuity in density, pressure and temperature that propagates at a well-defined speed u_s through a medium. We can understand the origin of such a discontinuity by considering the excitation of a series of high-amplitude pulsed compressions generated by

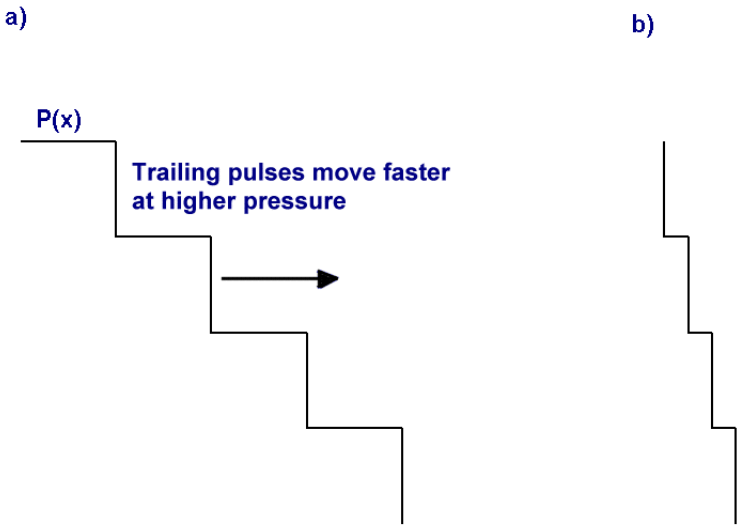

Figure 3: Propagation of a high-amplitude pressure waveform at early (a) and late (b) times.

applying a stair-step pressure waveform on the boundary of a medium. Figure 3a shows the pressure profile early in time as the compressions propagate into the medium at the sound speed. Because they move through regions of higher pressure and density, pulses produced later in time move faster according to Eq. 19. Eventually, they join with the initial pulses to produce a strong localized change in material properties (Fig. 3b). In other words, the characteristics of wave propagation in the material cause a broad, high-amplitude pressure waveform applied at the boundary to evolve to a sharp front.

Given the existence of a discontinuity, we can find relationships between material properties before and after passage of the shock by invoking conservation of mass, momentum and energy. Figure 4 shows a snapshot of a one-dimensional shock front moving in the $+x$ direction at speed u_s. The undisturbed medium to the right of the front has density ρ_0, pressure p_0 and internal energy U_0. We assume that the medium is initially at rest, or the average x velocity of *particles* in the medium is $u_{p0} = 0.0$. We can generalize the derivation by applying a coordinate transformation to a moving frame. The characteristics on the left-hand side of the shock are density ρ, pressure p and internal energy U. The shocked medium has a net average velocity u_p in the $+x$ direction consistent with conservation of mass and momentum. The quantity is usually called the *particle velocity*.

The total mass impinging on the shock from the right equals the total mass leaving to the left. The shock overtakes the undisturbed medium with velocity $-u_s$, so the rate of mass entering the shock per area is $\rho_0 u_s$. Material leaves the shock front with apparent velocity $(u_s - u_p)$, so the rate of mass leaving per area is $\rho(u_s - u_p)$. We can write the equation of mass conservation as

$$\rho_0 u_s = \rho(u_s - u_p). \tag{20}$$

Conservation of momentum implies that the time rate of change of particle momentum per unit area crossing the shock equals the difference in the force per area on each side of the shock. Initially, the particles have zero momentum. The time rate of charge is the rate of mass impinging on the shock times the final velocity: $(\rho_o u_s)u_p$. The momentum equation may be

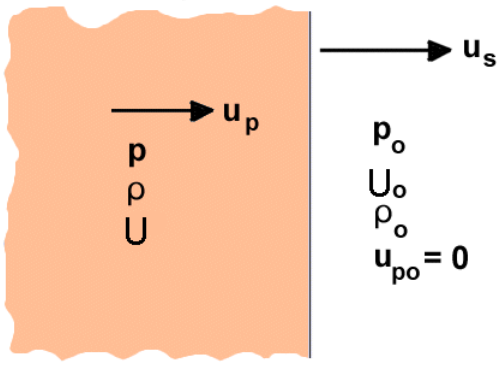

Figure 4: Change of quantities at a shock front.

written

$$p - p_0 = \rho_0 \; u_s \; u_p. \tag{21}$$

To express conservation of energy, we equate the rate of work performed by pressure force at the shock to the rate of change of kinetic plus internal energy for mass crossing the shock. In a time Δt, material occupying a volume per area of $u_s \Delta t$ on the upstream side of the shock changes to a volume per area $(u_s - u_p)\Delta t$ under the influence of a pressure p. The amount of work performed per area equals the pressure times the change in volume per area, or $p u_p \Delta t$. The rate of change of kinetic energy per area equals the mass entering the shock per area times the square of the final velocity or $\rho_0 u_s u_p^2$. The rate of change of the internal energy per area equals the mass rate entering the shock times the change in energy per mass, or $\rho_0 u_s (U - U_0)$. The equation of energy conservation is thus,

$$p u_p = \frac{1}{2} \rho_0 u_s u_p^2 + \rho_0 u_s (U - U_0). \tag{22}$$

Equations 20, 21 and 22 involve the known quantities p_0 and U_0 and the five unknown quantities ρ, p, u_s, u_p and U. With an additional equation, we could determine values for four of the unknown quantities in terms of one quantity and thereby generate a family of states that could be achieved by inducing shock waves in materials. The extra relationship is called the *equation of state* (EOS).

Equation 22 is often expressed in an alternate form called the *Hugoniot relation*. Solving for the change in internal energy gives,

$$U - U_0 = \frac{p u_p - \frac{1}{2} \rho_0 u_s u_p^2}{\rho_0 u_s}. \tag{23}$$

Equation 21 implies that the particle velocity is $u_p = (p - p_0)/\rho_0 u_s$. Substituting in Eq. 23, we find that

$$U - U_0 = \frac{p \; (p - p_0) - \frac{1}{2} (p - p_0)^2}{\rho_0^2 u_s^2}. \tag{24}$$

Combining Eqs. 20 and 21 gives the relationship

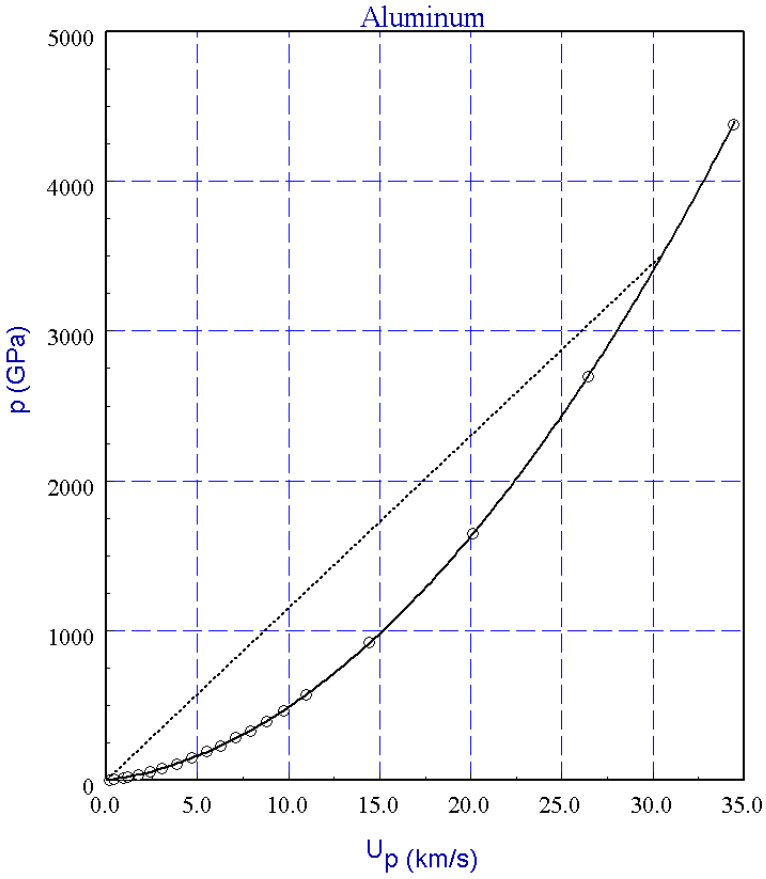

Figure 5: Hugoniot plot for aluminum. The marked points were calculated with the **KBView** program.

$$\rho_0^2 u_s^2 = (p - p_0)\frac{\rho\rho_0}{\rho - \rho_0}. \tag{25}$$

Finally, substituting Eq. 25 in Eq. 24 gives the Hugoniot relation:

$$U - U_0 = \frac{1}{2}\left(\frac{1}{\rho_o} - \frac{1}{\rho}\right)(p - p_0). \tag{26}$$

Given an equation-of-state, the shocked material quantities may be plotted as a function of a chosen independent variable. A useful curve is a plot of the change in pressure $(p - p_0)$ versus the particle velocity u_p. Figure 5 shows such a plot for aluminum generated from the table `ALUM3715.KBT` using the **KBView** program with $p_0 = 0.0$ Pa and $\rho_0 = 2700.0$ kg/m^3. The curve shows the range of possible final states resulting from a shock. The material changes rapidly from the initial state (origin) to a final state. A straight line on a Hugoniot plot connecting the initial and final states (dashed line in the figure) is called a *Rayleigh line*. On a p-u_p plot, the shock velocity may be inferred from the slope of the Rayleigh line. The equation for momentum conservation (Eq. 21) implies that

$$\rho_0 \; u_s = \frac{p - p_0}{u_p}. \tag{27}$$

The dashed line in Fig. 5 connects to a final state with $p = 3.401 \times 10^{12}$ Pa and $u_p = 3.0 \times 10^4$ m/s. The predicted shock velocity is 4.199×10^4 m/s. Note that the shape of the curve in the figure implies that u_s increases with the amplitude of the shock.

2.3 Detonation physics

Explosive materials release chemical energy at a very high rate. In the process of *detonation*, a solid or liquid explosive rapidly changes to a gas in a highly compressed state. During expansion the gas can perform a considerable amount of work. The quantity Q denotes the chemical energy released. Typical explosives have Q values of about 5 MJ/kG. Practical explosives have a high activation energy so that they do not spontaneously ignite. The required energy to initiate detonation is about 150 kJ/mole. For typical explosives the specific activation energy is about $U_a = 0.5$ MJ/kG. Ignition of an explosive material is usually performed by a detonator that generates a shock on the surface. The shock has sufficient amplitude to raise the internal energy by an amount exceeding U_a. The resulting rapid transformation of the material amplifies the shock which moves into adjacent regions. The process leads to a self-sustained detonation front that consumes the explosive material.

The detonation model used in **KB1** and **KB2** is straightforward[6]. Before detonation the properties of explosive materials are determined from the shock equation-of-state model discussed in Chap. 4. If the pressure in an element of explosive material exceeds a threshhold value p_{init}, the element detonates. At detonation the code augments the internal energy of the element by Q and subsequently determines the element pressure from the gamma law equation of state (Eq. 18). An underlying assumption is that the chemical reaction occurs rapidly in comparison to the propagation time for the detonation front.

The following parameters are required for a complete description of an explosive material in **KB1** and **KB2**:

ρ_0, the density of the solid material under ambient conditions (kg/m^3)

C_0, S_1 and S_2, parameters in the $u_s(u_p)$ relationship listed in Chap. 4.

p_{init}, the threshhold pressure for detonation (Pa).

Q, the specific energy released by the chemical reaction (J/kg).

γ, the constant for the gas equation-of-state.

The quantities ρ_0, Q and γ are discussed and listed in Appendix 1.

It is useful to review the equations for a one-dimensional detonation in a homogeneous material in order to understand the underlying physics and to define benchmark tests for the **KB1** and **KB2** codes. Figure 6 shows the geometry. A self-sustained front moves into an ambient explosive at a velocity u_d. The undisturbed material at rest has properties ρ_0, p_0, U_0 and $u_{po} = 0.0$. The gaseous material behind the front has density ρ, pressure p, internal energy U and a directed velocity u_p. We can determine unique values for the material state behind the front in terms of the properties of the explosive by applying conservation of mass, momentum and energy at the discontinuity. With the exception of the chemical energy released, the equations are the same as those derived in Sect. 2.2. The equation for conservation of mass is

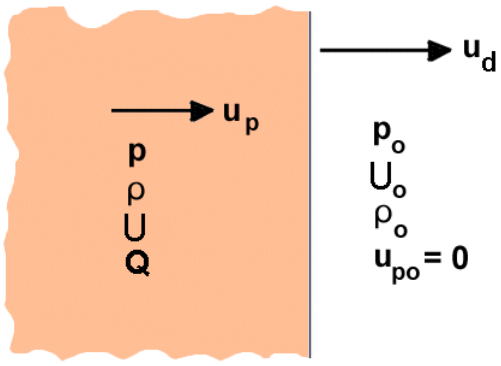

Figure 6: Quantities at a detonation front

$$\rho_0 u_d = \rho(u_d - u_p), \tag{28}$$

and conservation of momentum is given by

$$p - p_0 = \rho_0 u_d u_p. \tag{29}$$

To express conservation of energy, we include the specific chemical energy in Eq. 22:

$$U - U_0 = \frac{1}{2}u_p^2 + Q. \tag{30}$$

To simplify the equations, we assume that the initial pressure p_0 and internal energy U_0 are negligible compared to the values in the detonated state. Furthermore, we assume that the properties of the detonated material are governed by the gamma law equation-of-state:

$$p = (\gamma - 1)\rho_o U. \tag{31}$$

The momentum equation (Eq. 29) implies that following relationship for the detonation velocity:

$$u_d = \frac{p}{\rho_o u_p}. \tag{32}$$

We can combine Eqs. 28 through 31 to derive an expression for the material pressure in terms of the particle velocity,

$$p = \frac{1}{2}\rho_0(\gamma + 1)u_p^2 + \rho_0 Q(\gamma - 1). \tag{33}$$

Figure 7 shows a plot of Eq. 33 for Composition B ($\rho_0 = 1770.0$ kg/m^3, $Q = 6.270 \times 10^6$ J/kg and $\gamma = 3$). The plot represents an infinite set of possible states consistent with the explosive properties and conservation laws. The slope of a line connecting a point on the curve to the origin (dashed line in the figure) implies a value of the detonation velocity according to Eq. 32. Note that the dashed line illustrated presents an ambiguity. The same value of u_d corresponds to two different final states. The only possible unique state is shown by the solid line tangent to the curve, corresponding to the minimum value of u_d. This material state, the *Chapman-Jouguet point*[7, 8], represents the state of a detonation front. Note that the rationale

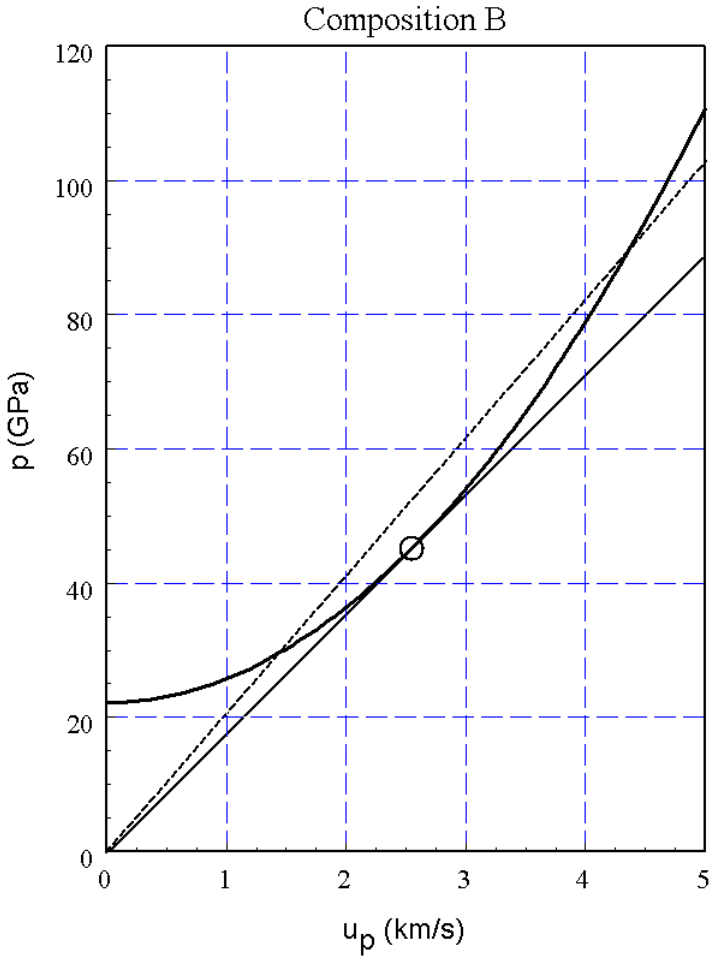

Figure 7: Determination of the Chapman-Jouguet point

for the Chapman-Jouguet condition is not intuitively obvious. A detailed discussion is given in J. Taylor, **Detonation in Condensed Explosives** (Clarendon Press, Oxford, 1952), 69-78.

We can find material properties at the Chapman-Jouguet point by combining Eqs. 32 and 33 to determine u_d in terms of u_p:

$$u_d = \frac{(\gamma+1)u_p}{2} + \frac{(\gamma-1)Q}{u_p}. \tag{34}$$

Setting $\mathrm{d}u_p/\mathrm{d}u_d = 0.0$ gives the particle velocity at the Chapman-Jouguet point as:

$$u_{pcj} = \sqrt{\frac{2Q(\gamma-1)}{\gamma+1}}. \tag{35}$$

Inserting Eq. 35 in Eq. 33 gives the Chapman-Jouguet pressure

$$p_{CJ} = 2\rho_o Q(\gamma-1). \tag{36}$$

Inserting the values u_{pCJ} and p_{CJ} into Eq. 32 gives the detonation velocity,

$$u_d = \sqrt{2Q(\gamma-1)(\gamma+1)}. \tag{37}$$

The parameters of Composition B used in Fig. 7 imply that $u_p = 2.50$ km/s, $p_{CJ} = 44.39$ GPa, and $u_d = 10.0$ km/s.

2.4 Two-dimensional hydrodynamics on a triangular mesh

The numerical treatment of the hydrodynamic equations in **KB2** is based on the division of the solution volume into small elements. The elements have a triangular shape so that they conform closely to boundaries in the initial system and can flex to follow changes in the geometry of the medium. Elements have a unique material identity that does not change during the simulation. On the other hand, the position, shape and size of elements may vary. The hydrodynamic quantities (pressure, density, temperature and internal energy) also vary. The finite-element approach is closely related to the Lagrangian viewpoint for finite-difference calculations. The calculation is referenced to materials rather than to a fixed coordinate system.

The computational approach in **KB2** has several advantages:

> The physical motion automatically refines the mesh – the code gives good results for systems that undergo substantial compression or expansion,
>
> The conformal mesh accurately represents curved or slanted material boundaries,
>
> The element-centered view helps in modeling complex processes like detonation.
>
> Unspecified boundaries automatically represent unconstrained material with free expansion.

On the other hand, **KB2** has drawbacks so it may not be practical for all problems. During a simulation it is essential to maintain the logical connections of the mesh. The implication is that elements that are initially neighbors must remain adjacent. Because **KB2** maintains continuity of phase space, it is not well-suited to systems that disassemble, cavitate or mix.

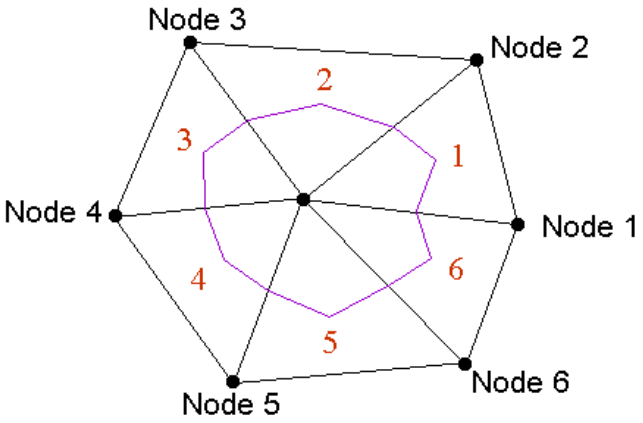

Figure 8: Elements and nodes surrounding an internal node.

Simulations terminate when elements are stretched to the breaking point (*i.e.*, logical inversion of a triangle). Similarly, it is difficult to represent systems with initially separated objects (*i.e.*, a shaped projectile striking a surface).

In **KB2** the term *element* refers to the area inside a triangle while the term *node* applies to the triangle vertices. Three quantities are associated with nodes: position ($[x, y]$ or $[[z, r]$), velocity ($[v_x, v_y]$ or $[[v_z, v_r]$) and mass (M). The remaining quantities are taken as properties of the elements: pressure (p), temperature (τ), density (ρ), internal energy (U) and artificial viscosity(($[w_x, w_y]$ or $[[w_z, w_r]$). The code solves equations of motion for nodes to infer changes in the element size and shape. The change in element volume is then used to update the hydrodynamic quantities. In the mesh created by the **Mesh** program, every internal node is surrounded by six elements as in Fig. 8. In the figure, elements and nodes surrounding the central node are labeled 1-6. The path shown in blue passes through the centers of lines connecting neighboring nodes and the centers-of-mass of the elements. The path encloses one-third of the element areas. We set the node mass M equal to the mass inside the path (one-third of the mass of the six elements). The element mass equals ρ multiplied by the element volume. The node masses are invariant because the element masses are conserved.

The force on a node arises from the pressure and artificial viscosity of surrounding elements. The total force on a node is determined from an integral of pressure over the surrounding surface shown in Fig. 8. After some algebra, the integration yields a simple and intuitive result. In planar geometry, the expression for pressure force (per length in z) is:

$$F_x = -\frac{1}{2}[P_1(y_1 - y_6) + P_2(y_2 - y_1) + P_3(y_3 - y_2) + P_4(y_4 - y_3) + P_5(y_5 - y_4) + P_6(y_6 - y_5)], \tag{38}$$

$$F_y = \frac{1}{2}[P_1(x_1 - x_6) + P_2(x_2 - x_1) + P_3(x_3 - x_2) + P_4(x_4 - x_3) + P_5(x_5 - x_4) + P_6(x_6 - x_5)]. \tag{39}$$

The quantities (x_i, y_i) are the coordinates of the surrounding nodes.

At each integer time step **KB2** determines the force components at a node from values of pressure and artificial viscosity in surrounding elements. The equation of motion is used to

determine new values of node velocities at the half-integer time step. The velocities are then used to advance the node positions to the next integer time step. The node positions are then used to find new element volumes in planar or cylindrical geometry. A new value of internal energy U can be determined from the change of volume and other possible processes (such as detonation). Finally, the new density ρ and internal energy can be used to determine the pressure through the equation-of-state for the element material. The procedure is applied to all elements and continues over subsequent time steps.

Although the method is simple in principle, there are several challenges in the practical application:

representing of applied pressures over arbitrary boundaries,

implementing symmetry boundaries (sliding surfaces),

maintaining good accuracy near the axis of cylindrical systems.

adding artificial viscosity contributions for arbitrary triangular elements.

organizing multiple materials and regions.

3 KB tables

The equation-of-state tables supplied with **KB** are based on data from the Los Alamos National Laboratory Sesame Library[1]. This unclassified library (described in Refs. [11] and [12]) has been widely distributed. The **KB** tables consist of text files tabulating pressure $p(\rho, \tau)$ and internal energy $U(\rho, \tau)$ as functions of density and temperature. One or more tables may be loaded into **KB1** and **KB2** to define material characteristics. In comparison to the Sesame Library, the **KB** tables have the following features:

Material tables are separated into individual files that may be ported to programs in any language or on any computer system.

All quantities have been converted to SI units.

Extraneous material has been removed to make the tables more compact.

The order for recording quantities in the tables has been modified for more convenient use in hydrodynamic codes.

A total of 145 tables have been included with the **KB** package. Some materials have several tables covering different ranges of density and temperature. The tables have names of the form

```
TANT3520.KBT
```

The suffix `KBT` denotes a text equation-of-state table in the format described in this section. The first four characters in the file prefix are an abbreviation for the material – the example corresponds to a table for tantalum. The last 4 characters denote the corresponding material number in the Sesame Library. Four materials have been included that are not in the library.

The tables `IGAS0001.KBT` and `IGAS0002.KBT` describe ideal gamma-law gases with $\gamma = 5/3$. They are useful for hydrodynamic benchmark tests. The table `IGAS0002.KBT` covers a much broader range of density and temperature than `IGAS001.KBT`.

The tables `HYDR0001.KBT` and `DEUT0001.KBT` describe hydrogen and deuterium in the gaseous and plasma states including the energy of ionization.

The tables may be viewed with a text editor. All files consist of a header and four tables. The header has the form:

```
*** Header
Material number:  7111
Rho0:  2.3500E+03
NRho:   100
NTemp:    23
```

The quantities have the following meanings:

[1]The **KB** Tables are translations of the public domain Los Alamos National Laboratory Sesame Tables. Although we have made efforts to ensure a faithful translation, Field Precision assumes no responsibility for the numerical or physical validity of the data.

Material number: number of the corresponding LANL Sesame Table

Rho0: usually the ambient material density. For some gases, this quantity equals the density of the solid or liquid form (kg/m^3).

NRho: the number of density values in the tables.

NTemp: the number of temperature values in the tables.

The first table contains the tabulated values of density (in kg/m^3). Each line consists of the value of I (the density index in FORTRAN format I5) and the corresponding value of density (format E13.5):

```
*** Table 1.  Rho(I) (kg/m3)
    1   1.8359E+01
    2   3.5029E+01
    3   5.1700E+01
    4   9.9288E+01
 ...
   98   1.1750E+07
   99   2.3500E+07
  100   4.7000E+07
```

The second table contains the values of J (the temperature index) and the temperature in ^{o}K (format I5, E13.5)

```
*** Table 2. Temp(J) (degrees K)
    1   0.0000E+00
    2   2.9012E+02
    3   5.8024E+02
   ...
   22   2.3210E+08
   23   3.7136E+08
```

The third table, $p(\rho, \tau)$, contains values of pressure (in Pa) at the tabulated density and temperature values (format E11.4):

```
*** Table 3. Pressure(I,J) (GPa)
 0.0000E+00
 3.4134E$-$27
 9.0019E$-$27
 2.4871E$-$26
 7.2005E$-$26
 1.7276E+04
  ...
 7.3426E+19
 1.0184E+20
```

Quantities are recorded in the following order with density as the inner loop and temperature as the outer loop:

```
DO J=1,NTemp
  DO I=1,NRho
     WRITE(P(I,J))
  END DO
END DO
```

The final table, $U(\rho, \tau)$, contains values of the material internal energy (in J/kg) at the tabulated density and temperature values. The order of recorded quantities in the same as for the pressure.

```
*** Table 4. Internal energy (I,J) (MJ/kg)
 0.0000E+00
 0.0000E+00
 0.0000E+00
   ...
 6.9994E+12
 6.9386E+12
 6.8065E+12
 6.6461E+12
 6.4076E+12
```

4 Shock equation-of-state

For many materials we do not have the full equation-of-state information represented by the **KB** tables. Fortunately complete information is not required in many applications. As an example, consider propagation of a shock. The conservation laws discussed in Sect. 2.2 limit the range of states that materials can attain. In this case, we can use a simplified equation-of-state that applies only to shock transitions. We must keep in mind that such a model may not provide an accurate description of how the material relaxes after the shock has passed. This limitation does not present a problem for modeling shock-detonated explosives. At detonation the solid explosive rapidly changes to a gas mixture that is well-described by a γ-law equation of state (Eq. 18).

An extensive database of material shock behavior has been generated from experiments. Usually the measured quantities are the shock velocity u_s and the material velocity u_p behind the shock. The relationship between these quantities for a wide variety of materials is well-described by the polynomial relationship,

$$u_s = C_0 + S_1 u_p + S_2 u_p^2. \tag{40}$$

Given Eq. 40 we can substitute in the equations of Sect. 2.2 to find all material quantities from any choice of the unknown: ρ, p, U, u_s or u_p. Measured data have been collected in several references[9, 15].

The **KB** package includes an extensive tabulation of shock equation-of-state data derived from Ref. [13]. The file `shockeos.xls` (in Excel format) contains values of the parameters C_0, S_1 and S_2 in Eq. 40 derived from least-squares fits for all materials where a sufficient number of data points were available. The parameters are also listed at the end of this chapter. All quantities are in SI units. Two additional quantities are included. The first, *Stdv*, is the standard deviation of measured values of u_s about the fitted curve. It indicates the variations in the experimental data. The second quantity, *upmax*, is the maximum measured value of u_p. Use of the fitted curve beyond this point involves extrapolation.

The quality of available data varies considerably. For example, Figure 9 shows the data points and fit for solid copper. As with most metals, the $u_s(u_p)$ curve is almost a straight line. Figure 10 shows an exception, the curve for antimony. Figure 11 shows data for the explosive Composition B. Understandably, fewer data points are available. There could be significant errors for extrapolations beyond $u_s = 1000$ m/s.

As described in Sect. 2.1, we need a function of the form $p(\rho, U)$ to close the hydrodynamic equations used in the **KB** codes. We can derive such a relationship for materials undergoing a shock transition by combining Eq. 40 with the equations of Sect. 2.1. The Hugoniot relation can be written

$$U - U_o = \frac{1}{2}\left(\frac{\rho\rho_o}{\rho - \rho_o}\right)(p - p_o). \tag{41}$$

Substituting for (p-p_o) from Eq. 2.8 gives

$$U - U_o = \frac{1}{2}\left(1 - \frac{\rho_o}{\rho}\right) u_s u_{p.} \tag{42}$$

The mass conservation equation implies that

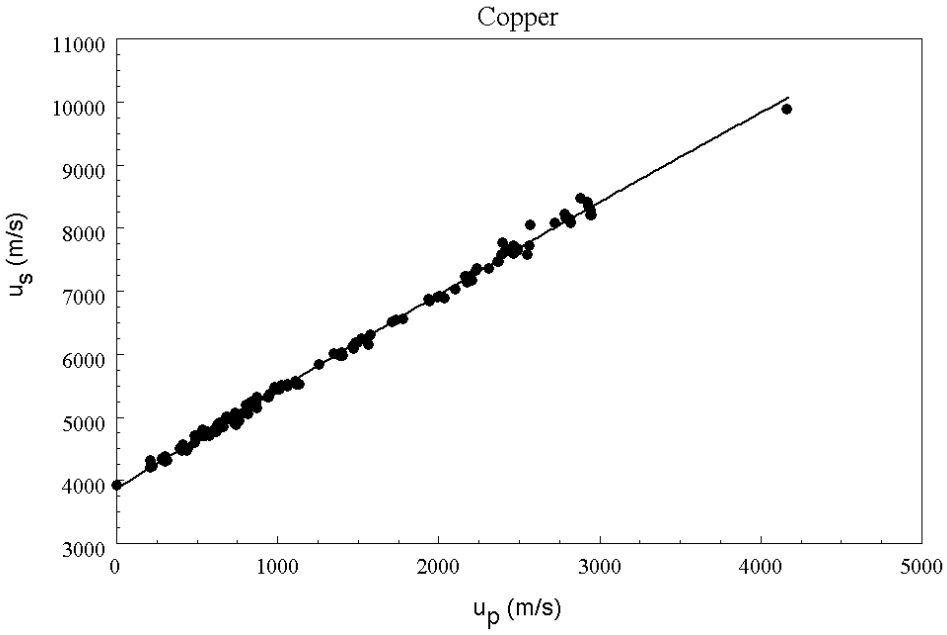

Figure 9: Least-squares fit to the data for copper in Ref. [13]

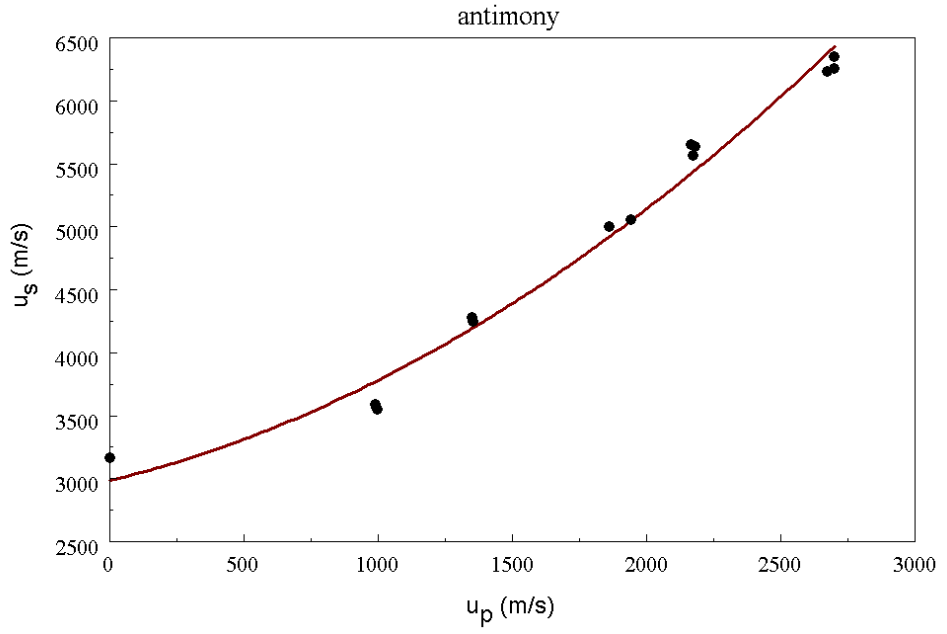

Figure 10: Least-squares fit to the data for antimony in Ref. [13]

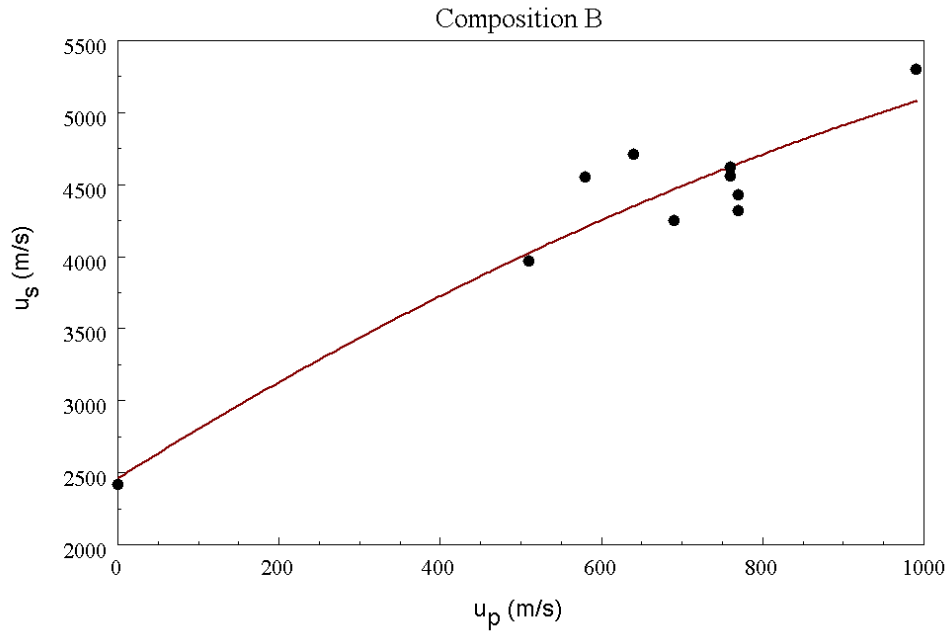

Figure 11: Least-squares fit to the data for Composition B in Ref. [13]

$$\frac{\rho}{\rho_o} = 1 - \frac{u_p}{u_{s.}} \tag{43}$$

Combining Eqs. 3.3 and 3.4,

$$U - U_o = \frac{1}{2} u_p^2, \tag{44}$$

or

$$u_p = \sqrt{2(U - U_o)}. \tag{45}$$

Given $u_{\rm p}$, we can find $u_{\rm s}$ from Eq. 3.1. Application of the energy equation (Eq. 2.9) gives an expression for the pressure:

$$p = \rho_o u_s \left(\frac{u_p}{2} + \sqrt{\frac{U - U_o}{2}} \right). \tag{46}$$

Equations 3.6 and 3.7 involve differences in internal energy, U-$U_{\rm o}$. The convention in **KB** is to take $U_{\rm o} \approx 0$ for materials described by the shock equation-of-state.

Another type of material model used in the **KB** codes is the gamma-law gas (Eq. 2.5). In this case, the pressure is given by

$$p = (\gamma - 1)\rho_o U. \tag{47}$$

5 KBView

KBView is an interactive program that uses the **KB** tables to determine and to display the properties of materials over wide ranges of density (ρ), temperature (τ) and pressure (p). **KBView** has the following capabilities:

Equation-of-state calculator to find $\rho(p,\tau)$, $p(\rho,\tau)$, $\tau(\rho,p)$, $U(\rho,\tau)$, $\tau(\rho,U)$ and $c_s(\rho,\tau)$, where U is the internal energy and c_s is the sound speed.

Parameter scans over a range of values of the types $\rho(p,\tau)$, $p(\rho,\tau)$, $\tau(\rho,p)$ and $U(\rho,\tau)$.

Plots and listings of isobars $[T(\rho)]$, isotherms $[p(\rho)]$ and isodensity lines $[p(\tau)]$.

Calculation of Hugoniot curves with plots and listings of $T(\rho)$, $P(\rho)$, $P(T)$, $P(u_{\rm p})$, and $u_{\rm s}(u_{\rm p})$, where $u_{\rm p}$ is the material speed behind a shock and $u_{\rm s}$ is the shock speed.

Calculation of isentropes with plots and listings of $p(\rho)$ and $U(\rho)$.

The program has several convenient features including: optional file listings of all calculations, automatic grids and scaling on plots, and hardcopy to any installed Windows printer. You can run `kbview.exe` directly or from `kb.exe`, the **KB** program launcher. For ease of use, **KBView** uses a set of practical units rather than the standard SI units used in the **KB** tables. Table 3 shows a comparison of units.

Table 3: Units used in **KBView** and **KB** tables

Quantity	KBView	KB table	SI convert
Density, ρ	gm/cm^3	kg/m^3	1000.0
Temperature, T	^{o}K	^{o}K	1.0
Pressure, P	GPa	Pa	10^9
Internal energy, U	MJ/kg	J/kg	10^6
Velocity, $u_{\rm p}$ or $u_{\rm s}$	km/s	m/s	1000.0

5.1 File menu

Figure 12 shows the **KBView** screen display. The program is a full-featured Windows utility with popup menus, a tool and status bar and an internal editor. When **KBView** starts only the *File* and *Help* menus are active. The analysis functions become active after a data file is loaded. The *File* menu contains the following commands:

LOAD MATERIAL

The first step in an analysis session is to load a **KB** material file. The program displays a dialog that lists files in the current directory with suffix `KBT`. Pick a file and click *Open*. You can change the working directory from within the dialog. After the material loads the program displays a box with information on the file. Click *OK* to continue. The **KB** tables contain the

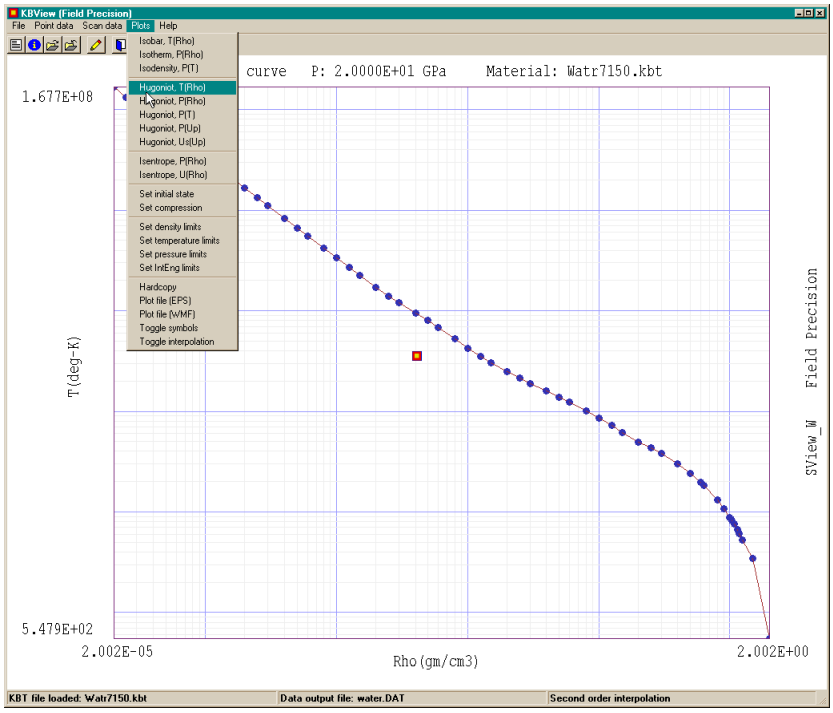

Figure 12: **KBView** screen

pressure and internal energy as functions of the material density and temperature. The message box shows the number of entries and the ranges of ρ and T. When you exit the dialog all menu functions are active. The first tool on the toolbar performs the *Load material* function. To see the functions of the other tools, suspend the mouse cursor over the tool until a description appears.

MATERIAL FILE INFO

If you want to check on parameter ranges in the current table, use this command to display the file information box.

OPEN DATA FILE

The analysis functions you perform in **KBView** may be recorded permanently in an text data file. Use this command to open a file to store information from subsequent operations. Enter a prefix (1-46 characters) for the file. Information will be written to a file `PREFIX.DAT` in the current directory until you 1) open a different file, 2) close the file with the *Close data file* command, or 3) exit **KBView**.

CLOSE DATA FILE

This command terminates file listings and closes the current data file. Be sure to close a data file before you attempt to *Edit* it.

EDIT FILE

This command brings up Windows editor for text files. You can view **KBView** data files or directly inspect **KB** tables.

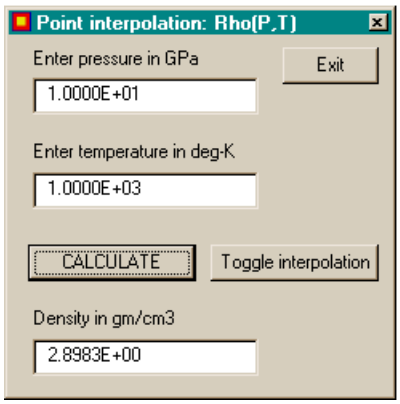

Figure 13: Point calculator

5.2 Point data menu

The commands in this menu call up a set of equation-on-state calculators that perform single-point interpolations on the **KB** tables (Fig. 13). A common application is to check whether a choice of ρ and τ for initial material conditions in **KB1** or **KB2** leads to valid interpolations for p and U.

Enter the two known quantities, press *Calculate*, and **KBView** displays the results using the current interpolation method. The *Interpolation* button toggles between first and second order interpolations. Click on *Exit* when you are finished. Note that the c_s (sound speed) calculation may be inaccurate at low temperatures where some of the tables are coarse. If a data file is open, **KBView** records calculator results. Note that the program also records **KB** table information in the listing file when the data file is opened or when a new material is loaded.

```
Point calculation of Rho(P,T)
      Pressure:   1.0000E+01 (Gpa)
   Temperature:   1.0000E+03 (deg-K)
    >> Density:   2.8983E+00 (gm/cm3)
```

There are six commands that control the type of calculation:

Rho(P,T)
P(RHO,T)
T(RHO,P)
U(RHO,T)
T(RHO,U)
Cs(RHO,T)

The default interpolation method is a least-squares fit of a second-order two-dimensional function. The first order function has reduced accuracy and a shorter calculation time.

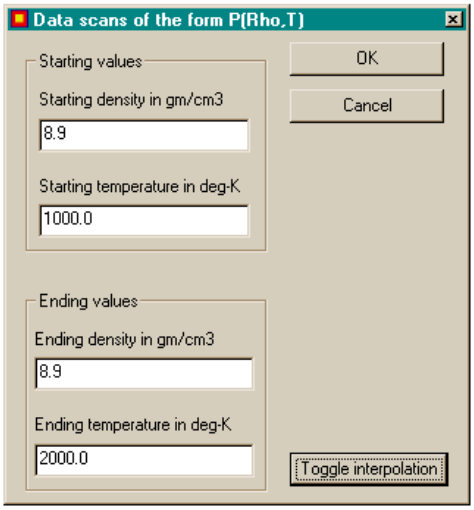

Figure 14: Input dialog for *Scan data* commands.

5.3 Scan data

The commands in this menu create scan listings of equation-of-state calculations of the following types: $\rho(p,\tau)$, $p(\rho,\tau)$, $\tau(\rho,p)$ and $U(\rho,\tau)$. When you choose one on these options the program displays a dialog box where you set limits for the independent variables (Figure 14). The program then determines the dependent variable for linear variations of the dependent variables over the ranges and makes a screen listing. **KBView** also records the information if a data file is open.

```
   --- Listing of P(Rho,T) ---
 Rho(gm/cm3)     T(deg-K)          P(GPa)
=========================================
8.900000E+00   1.000000E+03   3.152812E+01
8.900000E+00   1.066667E+03   3.192849E+01
8.900000E+00   1.133333E+03   3.233742E+01
8.900000E+00   1.200000E+03   3.275491E+01
8.900000E+00   1.266667E+03   3.319781E+01
8.900000E+00   1.333333E+03   3.361512E+01
8.900000E+00   1.400000E+03   3.403674E+01
8.900000E+00   1.466667E+03   3.446266E+01
8.900000E+00   1.533333E+03   3.475091E+01
8.900000E+00   1.600000E+03   3.521508E+01
8.900000E+00   1.666667E+03   3.571996E+01
8.900000E+00   1.733333E+03   3.626556E+01
8.900000E+00   1.800000E+03   3.685952E+01
8.900000E+00   1.866667E+03   3.744762E+01
8.900000E+00   1.933333E+03   3.806861E+01
8.900000E+00   2.000000E+03   3.872248E+01
```

The following commands appear in the *Scan data* menu:

RHO(P,T)

P(RHO,T)
T(RHO,P)
U(RHO,T)

Open a dialog to set scan ranges and then perform the requested number of calculations. Data is displayed on the screen and optionally to a listing file.

NUMBER OF POINTS
Changes the number of calculated points (Default: 25).

5.4 Plot menu

KBView generates several two-dimensional plots for hydrodynamic analyses. The plots are normally created on the screen, but can be directed to any hardcopy copy device supported by Windows or plot files in two formats: Encapsulated PostScript (EPS) or Windows Metafile Format (WMF). The *Plot menu* includes the following commands.

ISOBAR
ISOTHERM
ISODENSITY
The first three commands plot the following quantities:

Isobar: $\tau(\rho)$ at constant p.

Isotherm: $p(\rho)$ at constant τ.

Isodensity $p(\tau)$ at constant ρ.

The program prompts for a value of the constant quantity before each plot. Note that it may not be possible to perform the given interpolation over the full range of the table.

The next command set plots material properties behind a one-dimensional shock calculated from the Hugoniot equation.

$$\left(\frac{1}{\rho_0}-\frac{1}{\rho_1}\right)\left(\frac{P_1+P_0}{2}\right)=U_1-U_0. \tag{48}$$

The equation follows from conservation of mass, momentum and energy across the shock front. The quantities ρ_0, p_0 and U_0 are the initial density, pressure and internal energy of the material and the quantities ρ_1, p_1 and U_1 represent the state behind the shock. When a material is loaded, **KBView** fills arrays of values for quantities on the Hugoniot curve for a default initial state. The default state is calculated with ρ_0 equal to the normal density entry in the **KB** table and τ_0 equal to 300 ^{o}K. The program attempts to find values of p_1, τ_1 and U_1 through interpolations at each tabulated value of ρ. Depending on the initial state, the calculation may not be possible for all density entries. The conservation laws also give values for u_s (the shock velocity) and u_p (the velocity of the medium behind the shock called the *particle velocity*). The initial particle velocity of the medium is taken equal to zero. You can apply the results

to moving media by making a coordinate transformation. **KBView** updates the Hugoniot arrays under three conditions: 1) a new material is loaded, 2) the interpolation parameters are changed or 3) the initial state is changed.

The following commands plot Hugoniot curves with several choices of dependent and independent variables.

HUGONIOT, P(RHO)
HUGONIOT, T(RHO)
HUGONIOT, P(T)
HUGONIOT, P(UP)
HUGONIOT, UP(US)

The next set of commands initiates plot of isentropes. Isentropic curves follow changing material properties from an initial state along a path that preserves entropy. In other words, the process is reversible. **KBView** computes *isentropic compressions* where the density changes from an initial value ρ_0 to a final density $C_f\rho_0$ at constant temperature. Here, C_f is a compression factor with default value $C_f = 100$. The equation for an isentropic compression is

$$dU = -p\ d(1/\rho) = p\ d\rho/\rho^2. \tag{49}$$

KBView solves the equation and fills isentrope arrays using table interpolations and a two-step integration method. The integration starts from the initial material state and proceeds to the final compressed density. Ideally the temperature remains close to τ_{init}. The arrays are updated under the same circumstances as the Hugoniot arrays.

The following commands plot isentropic compression curves with two choices of dependent and independent variables.

ISENTROPE, P(Rho)
ISENTROPE, U(RHO)

The final set of commands control plot parameters and initiates hardcopy output.

SET INITIAL STATE
Hugoniot and insentrope calculations start from an initial state of the material. Use this command if you want to change the default values. The program displays the EOS calculator (Figure 5.2). Supply values of ρ_0 and τ_0. You can use the *Calculate* button to check that the values give a valid interpolation for the pressure. Change the interpolation method if necessary. Click on *Exit* to set the values.

SET COMPRESSION
Set the quantity C_f to define the density range of the isentrope calculation.

HARDCOPY
PLOT FILE (EPS)
PLOT FILE (WMF)
These commands initiate output of the current screen plot. They will not function unless you have created a screen plot. The *Hardcopy* option sends the plot to the Windows default printer. If you want to pick a different printer driver, you must change the Windows default. You can can call up the *Control Panel* while the program is operating. For plot files, **KBView** prompts for the file prefix and creates the file in the current directory. PostScript files have the suffix `EPS` and Windows Metafiles have the suffix `WMF`.

5.5 Help menu

You can display a PDF version of this manual within the program using the *KB manual* command or tool. The command calls up your default browser and loads the file `kb.pdf`. This file should be located in the same directory as the executable **KB** programs.

6 KB1

6.1 Introduction

KB1 performs hydrodynamic simulations of materials at high temperature and pressure. The code handles one−dimensional problems in planar, cylindrical and spherical geometries. **KB1** uses element-based methods based on difference equations derived from integral conservation relationships. The mathematical foundation of **KB1** was described Chap. 2. Three programs are involved in the one-dimensional simulations:

KB1: main simulation program controlled by an input script.

KB1V: interactive graphical post-processor for data files (spatial variations of quantities at specified times)

Probe: plotting and oscilloscope utility used to inspect and to plot **KB1** history data.

Table 1 summarizes physical units used in **KB1** and **KB1V**. In the remainder of this section we shall walk through an example to introduce you to the program.

Table 4: Physical units for the **KB1** programs

Quantity	**KB1**: internal operations, data and history files	**KB1V** and **Probe**
Density	kg/m^3	gm/cm^3
Position	m	cm
Pressure	Pa	GPa
Temperature	^oK	^oK
Internal energy	J/kg	MJ/kg
Velocity	m/s	km/s

To illustrate the sequence of operations in a **KB1** run, we shall follow the example `SEDOV`, described in Sect. 12.4. The first step is to collect data that will be used by the program. Ensure that the files `SEDOV.KIN` and `IGAS002.KBT` are located in the working directory. Run the program launcher `kb.exe`. If necessary, use the *Data directory* command to specify the working directory. Click the button next to **KB1** to run the program. Pick the *Start run* tool or click on the *Run/Start run* menu options. In the dialog, pick the file `SEDOV.KIN`. The program loads data and starts the calculation. It should take about 1-2 minutes to finish.

The program uses and creates different types of files. Go to the *File* menu in **KB1**, choose *Edit KIN file*, and then choose `SEDOV.KIN` in the dialog. The program runs a full-featured Windows editor and loads the file (shown in Table 5. It is a text script that performs several functions:

Table 5: Contents of the file SEDOV.KIN.

```
* --- CONTROL ---
  TITLE: Sedov spherical blast wave
  GEOMETRY: SPHERE
  INTERPORDER: FIRST
  DT: 0.25E-9
  DTCHANGE 0.5E-6 2.5E-9
  TMAX:  5.01E-6
* --- MATERIALS ---
  MATERIAL 1 KBT IGAS0002
*  MATERIAL 1 GAMMA 1.66667
* --- GEOMETRY ---
  REGION  1  1  0.0000 0.002 5
  REGION  2  1  0.0020 0.060 90
* --- REGIONS ---
  HYDINIT 1  0.1000 2.135E7
*  HYDINIT 1  0.1000 1.84E11
  VISCOSITY 1 2.50
  HYDINIT 2  0.1000 0.001
*  HYDINIT 2  0.1000 0.000
  VISCOSITY 2 2.50
* --- DIAGNOSTICS ---
  DTIME: 0.25E-6
  PROBESTEP: 25
  SETPROBE: 2
  SETPROBE: 70
*
ENDFILE
```

Sets control parameters such as the time step or system symmetry.

Defines the geometry by dividing the solution space up into *regions* with common material characteristics.

Specifies material models to be associated with the regions.

Sets initial conditions and driving terms.

Controls diagnostic output.

Close the edit window and choose the command *Edit file* from the *File* menu. In the dialog, pick IGAS0002.KBT. This file provides the equation-of-state information required to solve the hydrodynamic equations. Note that the file is in text format. You can incorporate the data into your own programs. Chapter 3 gives detailed information. An inspection of the working directory shows that the program has created four output files: SEDOV.KLS, SEDOV.P01, SEDOV.P02 and SEDOV.KPL. Open SEDOV.KLS using the *Edit KLS file* command. This listing file

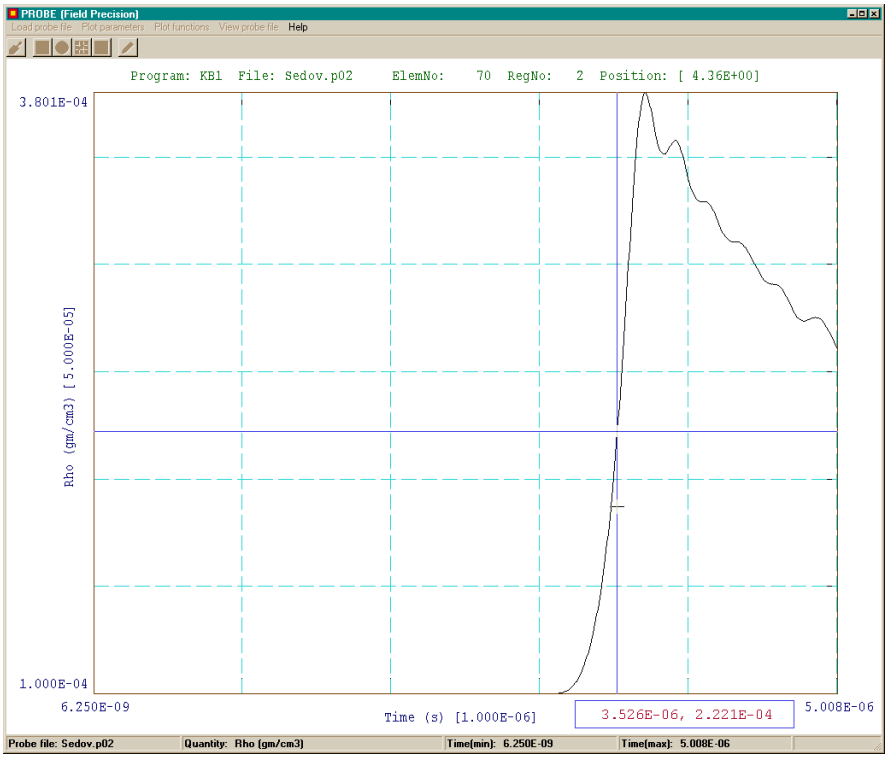

Figure 15: **Probe** program display.

contains run information and extensive quantitative data. The bulk of the file consists of *data dumps*, listings of hydrodynamic quantities at all points in space at times specified by the input script file. The file `SEDOV.KPL` contains the data dump information in binary format. This file is used by the **KB1V** program for interactive analyses and plots. Finally, check `SEDOV.001` using the *Edit file* command. This file contains history information, a record of hydrodynamic quantities as a function of time in a given element. A **KB1** run may create several history files for different elements. You can use this information directly in your own analyses or use the **Probe** program to create plots and check values.

Next, run **Probe** from the **KB** program launcher. Click on *Load probe file* and pick *SEDOV.P02* in the dialog. The message box shows information on the file. Click *OK* to continue. Under *Plot parameters*, click on *Pick plotted quantity* and choose *density*. You should see the plot of Fig. 15. Under *Plot functions*, choose *Oscilloscope mode*. By moving the mouse, you can measure points on the plot. Click the right mouse button to return to the program. Chapter 10 gives a detailed description of the program capabilities.

Finally, run **KB1V** from the **KB** program launcher. Under *File* click on *Load plot file*. In the dialog, choose *SEDOV.KPL* and click *OK*. Under *Spatial plots*, choose *Set included plots*. The listing in the dialog shows that dumps were recorded at intervals of 0.25 μs. You can turn plots *ON* and *OFF* by clicking on them. Activate the plots for 0.50 μs, 1.00 μs, 1.50 μs and 2.00 μs and click on *OK*. Under *Spatial plots*, choose *Screen plot*. You should see the display of Fig. 16. The **KB1V** manual describes other features of the program.

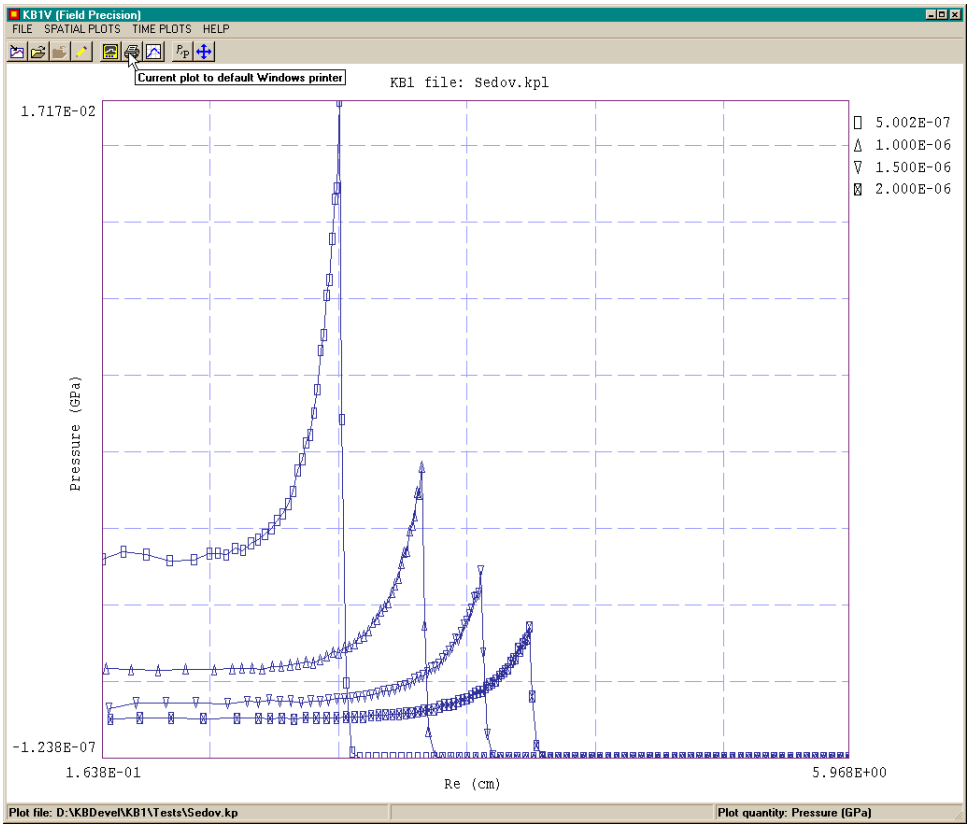

Figure 16: **KB1V** program display.

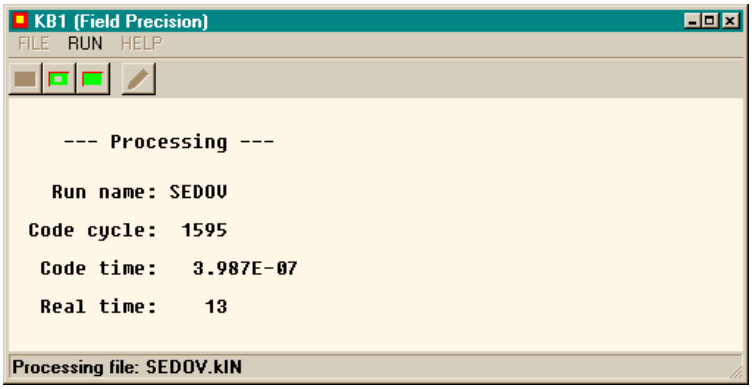

Figure 17: **KB1** screen display, interactive mode.

6.2 Running KB1

The program `kb1.exe` can run in two modes: 1) an interactive Windows application and 2) an autonomous task run from the command Prompt, usually under batch file control. We shall first discuss the interactive mode. There are several ways to start `kb1.exe`: click the entry on the **KB** program launcher, set up a shortcut on the Windows desktop or start menu, double-click on the program in Windows Explorer, or use the *Run* option on the start menu. In all cases, the window shown in Figure 17 appears. Entries in the popup menus have the following functions.

EDIT KIN FILE
EDIT KLS FILE
EDIT FILE

The program has a built-in Windows editor that can be used to inspect input and output text files. The difference between the commands is the choice of files displayed in the opening dialog. Files with suffix `KIN` are **KB1** input files. Files with suffix `KLS` are output listing files which contain run information and data dumps. Changing directories in the dialog does not change the working directory of the program. Close the editor to continue **KB1** operation.

START RUN

This command initiates a **KB1** calculation. The dialog displays all files in the current working directory with the suffix `KIN`. Pick a file and click *OK.* The run proceeds if the command script is syntactically correct and the required input data files are present. The data window (Fig. 17) shows the run identifier, the number of cycles (time steps) processed, the simulation time, and the actual time elapsed.

PAUSE RUN

KB1 is a number cruncher that can occupy the full resources of your computer. As a result other programs may run slowly. If you need to perform a critical task in the middle of a **KB1** run, you can pause the program. Click the *Resume* button to continue with no loss of data.

STOP RUN

The *Stop run* command is useful if a run is taking too long or you want to check output from the first part of an extended run. This command prompts for confirmation, closes all files and stops the program. Previously recorded data dumps and probe information will be available.

KB MANUAL

Displays this document if it is located in the same directory as `kb1.exe`.

You can run **KB1** as an autonomous program from the command prompt by supplying the prefix of the input file as a command line parameter. For example, suppose that the program is in the directory `\fieldp \kb` and that the input file `SEDOV.KIN` is in the directory `\workdir`. Type

```
\fieldp\kb\kb1 \workdir\sedov <Enter>
```

This capability is useful if you want to prepare a batch file for a set of extended runs. For example, the following file would perform five calculations with no operation intervention:

```
REM Cylindrical detonators\\
REM Variation of initiator radius\\
START /B \fieldp\kb\kb1 \workdir\cyldet01
START /B \fieldp\kb\kb1 \workdir\cyldet02
START /B \fieldp\kb\kb1 \workdir\cyldet03
START /B \fieldp\kb\kb1 \workdir\cyldet04
START /B \fieldp\kb\kb1 \workdir\cyldet05
REM Job completed
```

6.3 Geometry and mesh conventions

The basis of the finite-element approach is the division of the solution volume into many small pieces or *elements*. In the limit where the element size is small compared to the scale length for significant variations, the continuous equations of hydrodynamics reduce to a set of coupled linear equations that can be solved easily on a computer. The division is carried out so that each element has a unique material identity. In other words, the boundaries between elements are chosen so that they lie along the boundaries between different types of materials in the solution space. Another important term is *node*. In the one-dimensional solutions of **KB1**, a node is the boundary between elements. (In the two-dimensional solutions of **KB2** nodes are the intersection points of element boundaries.) To solve the hydrodynamic equations it is convenient to associate some quantities with elements (usually material properties and hydrodynamic state) and others with nodes (Table 6).

Figure 2 shows the division of a volume into elements for a **KB1** solution. The program handles systems with planar, cylindrical and spherical symmetry. In the three modes elements represent slabs, cylindrical shells, or thin spherical shells. In planar geometry slabs move in x and have infinite lengths in y and z. In cylindrical geometry shells move in r, are symmetry in ϕ, and have infinite length in z. In spherical geometry shells move in r and have symmetry in ϕ and θ. The thickness of elements need not be uniform in **KB1** solutions. Elements have indices in the range 1 to $N_{\rm e}$, while nodes are labeled from 0 to $N_{\rm e}$. With this convention Element n is bounded by nodes n-1 and n.

There are two other terms that apply to the organization of elements: *Material* and *Region*. The *material model* specifies the equation-of-state applied to an element. For given values of density and internal energy, the material model gives the corresponding pressure (and temperature for materials represented by **KB** tables). Section 6.7 describes the available options. Up to 20 material models may be defined for a **KB1** run. The quantity *MatNo* (an integer in the range 1 to 20) specifies the material model associated with the element. Elements are grouped into *Regions* (layers) that share common properties. Up to 12 *Regions* can be defined in a **KB1** run. All elements in a *Region* have the same material number. The number is assigned to the *Region*, and then all included elements are marked accordingly. Two separated or adjacent regions may use the same material model but may have different initial properties (*i.e.*, hydrodynamic state, velocity, element thickness, artificial viscosity coefficient,...). Table 6

Table 6: **KB1** quantities

Type	Quantity	**Definition**
Node	x[n]	Boundary between Elements n and n+1 (m)
	v[n]	Velocity of node n (m/s)
Element	**MatNo**[n]	Material number
	RegNo[n]	Region number
	Rho[n]	Density (kg/m^3)
	Press[n]	Pressure (Pa)
	Temp[n]	Temperature (^{o}k), KBT materials only
	Epsi[n]	Internal energy of Element n (J/kg)
	Mass[n]	Invariant mass (kg), internal program use
	WVis[n]	Artificial viscosity (Pa), internal use
	Detonated[n]	Detonation state, explosive materials only
Material	**Type**[i]	KBT, Void, ShockEOS, Gamma, Explosive
	MatPrefix[i]	KBT table name such as ALUM3715, (KBT)
	DBounce[i]	Minimum element thickness (m), (Void)
	C0[i],**S1**[i],**S2**[i]	Shock EOS parameters
	PInit[i]	Ignition pressure (Pa), (Explosive)
	Q[i]	Energy of detonation (J/kg), (Explosive)
	Initiated[i]	Detonation status at t = 0, (Explosive)
Region	**NMat**	Material number
	RI[j]	Initial inner radius (m)
	RO[j]	Initial outer radius (m)
	NElem[j]	Number of elements
	VInit[j]	Initial velocity (m/s)
	RhoInit[j]	Initial density (kg/m^3)
	PressInit[j]	Initial pressure (Pa)
	EpsiInit[j]	Initial internal energy (J/kg)
	TempInit[j]	Initial temperature (^{o}K), KBT materials only
	CVis[j]	Artificial velocity coefficient

Table 7: KB1 input and output files

Name form	I/O	Function	Format
`FPrefix.KIN`	Input	Script controls operation of the program	Text
`PressName`	Input	Table of waveform values for an applied pressure	Text
`KBTName.KBT`	Input	Equation-of-state table	Text
`FPrefix.KLS`	Output	Listing file, run information and data	Text
`FPrefix.KPL`	Output	Data dumps for **KB1V** analyses	Binary
`FPrefix.P01`	Output	One or more probe files, temporal information for a given element	Text

lists the quantities used in **KB1** to characterize nodes, elements, materials and regions. The quantities are divided into three classes:

1. may be set directly in the input script file (**bold**),
2. calculated by the program and recorded int the listing file (standard), and
3. calculated by the program and used internally (italic).

6.4 Structure of the input script

KB1 may use and create several types of files. Table 3 summarizes the function and format of different files. In this section and the following ones, we shall concentrate on the preparation of input files to control the run and to supply data. The input script is the fundamental control file required for all **KB1** runs. In is an text file that consists of a list of commands with parameters, similar to an interpreter program. The main difference is that the commands may appear in any order – the program sorts out the logic before proceeding to execution. The command file must have a name of the form `FPrefix.KIN`, where `FPrefix` is any valid DOS name from 1-46 characters in length. The script and other input files for equation-of-state data and pressure waveform information should be in the same directory. In the batch file mode the program is run with a command like

```
ProgDir\KB1 DataDit\FPrefix
```

where *ProgDir* represents the path to the executable files and *DataDir* is the path to the input files. In the interactive mode, you can use standard Windows file selection dialogs to change directories and pick a script.

Table 5 shows a sample input script. The file may contain command, comment and blank lines. A command line consists of a keyword and one or more parameters. Commands may

appear in any order because **KB1** sorts and processes information after all commands are read. You can enter commands and parameters in upper or lower case. Comment lines must begin with '* ' (asterisk-space). Commands and parameters may be indented. The program ignores spaces and other delimiters. The following are valid delimiters.

```
Space: ' '
Comma: ','
Colon: ':'
Equal sign: '='
Tab character
Left parenthesis: '('
Right parenthesis: ')'
```

Command input terminates with the *EndFile* statement. The command signals that input information is complete and **KB1** should begin execution. You can include descriptive text in any format after *EndFile*.

Commands fall into seven categories:

Controls: set general properties like the maximum run time.

Materials: define material models to be associated with regions and elements.

Geometry: define the dimensions and divisions of regions.

Regions: set region properties, such as the initial velocity or hydrodynamic state.

Diagnostics: control how much information is written to the listing, plot and probe files.

The following sections cover input script commands in detail. *Control* commands are reviewed in Section 6.5. Section 6.6 discusses the preparation of files to define applied pressure waveforms. Commands to define material properties are presented in Sect. 6.7, while Sect. 6.8 concentrates on explosive materials. *Geometry* commands are covered in Sect.6.9 and *Region* commands in Sect. 6.10. Section 6.11 reviews *Diagnostic* commands.

6.5 Control commands

Control commands may appear anywhere in the script file, although it is good practice to group them at the beginning. This section shows each command in symbolic form and also as it might appear in the script. The first two commands are required.

GEOMETRY [Rect, Cylin, Sphere]
GEOMETRY Cylin
This command sets the symmetry of the one-dimensional calculation. The single is the string *Rect*, *Cylin* or *Sphere*.

TMAX TMax
TMAX 5.75E-6
Sets the maximum run time. Specify the value in seconds.

TITLE Run title string
TITLE Ignition of TNT rod (small ignitor)
The title string (up to 60 characters) is useful for archiving a run and appears in plots created by **KB1V**.

SAFETY Safety
SAFETY 5.0
KB1 can pick a time step automatically for simple runs where there are no abrupt changes in quantities, such as collisions between regions. This command sets a safety factor for estimating a stable time step from the instantaneous element properties. Higher numbers are more conservative. Lower numbers reduce the run time at the risk of a numerical instability. Supple a single real number. The default value is 10.0.

NCHECK NCheck
NCHECK 50
Sets the number of program steps between recomputations under automatic time step control. Supply an integer value. The default is $NCheck = 5$.

DT Dt
DT 1.0E-09
This command sets the value of the initial time step and disables automatic time step selection. You may need to experiment to find a value of *Dt* that gives numerical stability with an acceptable run time. Supply a real-number value in seconds.

DTCHANGE TChange DtNew
DTCHANGE 5.0E-06 2.5E-09
The time step *Dt* changes to the value *DtNew* at time **TChange**. This command allows you to fine-tune the program for difficult simulations. For example, if a slab accelerates smoothly and then abruptly collides with another slab, you could use a long time step initially and then shorten it just before the collision. Another reason to lower *Dt* to handle the convergence of a shock on the axis of a cylindrical or spherical system. The *DTChange* command over-rides values set by the *Dt* command or automatic step selection. Supply two real-number parameters, both in seconds. The first (*TChange*) is the approximate time at which the change should occur, and the second (*DtNew*) is the new value of the time step.

INTERPORDER [First, Second]
INTERPORDER First
This command controls the type of interpolations performed for using **KB** tables. First order interpolations are generally sufficient for shock solutions at high temperature or pressure. Second order interpolations increase the run time significantly, but may be necessary to achieve accuracy in simulations where there are small changes of density or pressure. This command has no effect for *Void*, *ShockEOS*, *Gamma* and *Explosive* materials. The default type is *First*.

ERRSTATUS [All,Partial,None]
ERRSTATUS Partial
KB1 may perform millions of interpolations in runs with **KB** table materials. The operations are of the form $\tau(\rho, U)$ and $p(\rho, \tau)$. This command controls how the code responds when it detects an interpolation error. Errors in $\tau(\rho, U)$ may occur if the material is near ambient temperature and if the **KB** table has widely-spaced values at low temperature. In this case, there is little error introduced if we simply set the temperature equal to the initial value for the region if an error is detected. In the *Partial* option, the program ignores errors of the type $\tau(\rho, U)$, but terminates following an error in $p(\rho, \tau)$. In the *All* option, the program stops with an error message for any interpolation error. In the *None* option, the program ignores all interpolation errors. This option is useful mainly for debugging. This command has no effect for *Void*, *ShockEOS*, *Gamma* and *Explosive* materials. The default type is *Partial*.

FIXBOUND [Inside,Outside,Both,None]
FIXBOUND Inside
This command clamps the position of a node so that it does move during the run. For example, we could apply the condition to a boundary in a planar simulation to model one half of a symmetric system. Another application is representation of an ideal containment shell for a detonating gas. The string parameter options have the following meanings.

Inside: clamp the solution boundary at x_{min} or r_{min}.

Outside: clamp the boundary at x_{max} or r_{max}.

Both: clamp both boundaries.

The default is *None*.

6.6 Applied pressure waveforms

There are three ways to drive shock hydrodynamic solutions in **KB1**: setting initial velocities between colliding regions, detonating explosives, and applying a time-dependent drive pressure. This section explains how to define a time-dependent pressure waveform that acts at one or both of the solution boundaries. The controlling command has the following form:

PRESSURE TabName [Inside,Outside]
PRESSURE LinDrive.PRS Outside
Two *Pressure* commands may appear in the input script to define applied pressure waveforms at the inside and outside boundaries. There are two string parameters. The first gives the full name of a tabular function file in the current data directory. The file format is described below. The options for the second parameter have the following meanings.

Inside: apply the pressure at the solution boundary at x_{min} or r_{min}.

Outside: apply the pressure at the boundary at x_{max} or r_{max}.

Arbitrary time variations of pressure may be specified with tabular functions, text files that contain up to 256 data lines. Each data line contains two real numbers separated by spaces or other valid delimiters (see Sect. 6.4). The first number in each line is the time (in s) and the second number is a corresponding value of the pressure (in Pa). The time interval need not be uniform. For example, you may want to cluster values near a time when there is a sharp transition of pressure. The *EndFile* command marks the end of data entry. Tables may also contain comment lines starting with '* ' (asterisk-space) and blank lines. Table 8 illustrates a normalized pressure table.

KB1 finds interpolated values using a cubic spline interpolation of the data. This method is very flexible, but may give unexpected results for noisy or inaccurate data. For this reason, the program writes a test series of 50 interpolations uniformly spaced over the time interval 0.0 to *TMax* in the listing file.

An alternate form of the *Pressure* command allows you to add multiplying factors to normalized tables.

PRESSURE TabPrefix [Inside,Outside] TMult PMult
PRESSURE LinDrive.PRS Outside 1.0E-06 25.0E09

With this command you can maintain a library of normalized waveforms, using multiplication factors to apply them to different simulations. Note that the test interpolation listing shows values as they will be used in the program. There are two string and two real-number parameters. The first string gives the full name of a tabular function file in the current data directory. The options for the second string parameter have the following meanings.

Inside: apply the pressure at the solution boundary at x_{min} or r_{min}.

Outside: apply the pressure at the boundary at x_{max} or r_{max}.

The first real-number parameter is a multiplication factor for time values. The values used in the program are the table values multiplied by *TMult*. The second real-number parameter is a multiplication factor for the pressure values.

6.7 Standard material properties

Chapter 2 covered the material models used in **KB1** and **KB2.** It is important to note that the programs are useful for shock phenomena at very high temperatures and pressures. The current versions do include support for elastic or inelastic material strength and do not include effects of energy transport by thermal conduction or radiation. The programs use five models for the hydrodynamic properties of materials. They differ in how element pressure is inferred as a function of density and internal energy.

Table 8: Tabular function to define a variation of pressure

```
* Normalized smooth step function
* Rise to 1.0 at time 1.0
* ==============================
       0.00000        0.00000
       0.05000        0.00616
       0.10000        0.02447
       0.15000        0.05450
       0.20000        0.09549
       0.25000        0.14645
       0.30000        0.20611
       0.35000        0.27300
       0.40000        0.34549
       0.45000        0.42178
       0.50000        0.50000
       0.55000        0.57822
       0.60000        0.65451
       0.65000        0.72700
       0.70000        0.79389
       0.75000        0.85355
       0.80000        0.90451
       0.85000        0.94550
       0.90000        0.97553
       0.95000        0.99384
       1.00000        1.00000
       1.05000        1.00000
       1.10000        1.00000
       1.50000        1.00000
       2.00000        1.00000
       5.00000        1.00000
      10.00000        1.00000
      20.00000        1.00000
      50.00000        1.00000
     100.00000        1.00000
ENDFILE
```

KBT Materials. For these materials the programs use the **KB** tables to find both pressure and temperature of the material (Chap. 3). The *KB* table model has several advantages compared to the *Gamma* and *ShockEOS* models:

- It includes effects of phase changes in materials.
- It gives information on temperature as well as density, pressure and specific energy.
- It correctly represents both shock compression and subsequent expansion of materials.

The disadvantage is that the interpolations require more run time than the simple formula evaluation of the *ShockEOS* and *Gamma* models.

Shock EOS materials. The shock equation-of-state model gives useful approximations for materials that are not covered by the **KB** tables. The model yields changes in pressure as a function of density and internal energy with the assumption that material states lie on the shock Hugoniot curve. Chapter 4 gives detailed information. The model is applicable to materials undergoing shock compression, but it does not provide an accurate representation of subsequent expansion.

Gamma law materials. Many gases follow the law $p = (\gamma - 1)\rho_o U$ over a wide range of density and pressure. If applicable, the model has two advantages over interpolations on the **KB** tables.

- There are fewer numerical operations, leading to shorter run times.
- There is less chance of an interpolation error under extreme conditions.

The gamma law model is useful to avoid numerical instabilities in treating materials with very high density compressions, such as a gas entrapped between colliding solid regions.

Explosive materials. Explosive materials use both the *ShockEOS* and *Gamma* models. The shock equation-of-state applies to the solid or liquid materials before detonation. An element of explosive material detonates if it is subjected to a shock that raises the pressure above a critical value. At detonation, the density is unchanged while the internal energy increases by Q (the specific energy of detonation). For subsequent times the increased pressure is calculated from the gamma law model.

Void Materials. A void is a single-element region that occupies the space between initially-separated material regions. Voids are included because the finite-element method requires continuity of the solution volume.

Voids have a simple equation of state. The pressure is given by:

$$\begin{aligned} P &= 0.0, \quad (W_e > D_v) \\ P &= P_v \left(\frac{D_v}{W_e} - 1.0\right). \quad (W_e \le D_v) \end{aligned} \tag{50}$$

In the equations, W_e is the current width of the void element. The parameters P_v and D_v are defined in the void material command.

The following commands set the properties of a numbered material model. You can define up to 20 material models. A model may be associated with several regions.

MATERIAL MatNo KBT TabName
MATERIAL 5 KBT ALUM3715

This command loads the **KB** table `TabName.KBT` and assigns it as material model *MatNo*. The table must be in the current directory. The initial hydrodynamic state of the material may be set individually in different regions. The parameter *MatNo* is an integer in the range 1-20 to identify the material model. The string *KBT* designates that the equation-of-state will be determined from interpolations on a **KB** table. The string *TabName* (1-46 characters) is the prefix of the **KB** table.

MATERIAL MatNo SHOCK C0 S1 S2
MATERIAL 4 SHOCK 2.985E3 0.5148 2.814E-4

This command defines material *MatNo* as a *ShockEOS* material and sets the relationship between u_s (shock velocity) and u_p (particle velocity) as defined in Chap. 4. The initial density may be set individually in different regions. The initial pressure equals zero. The parameter *MatNo* is an integer in the range 1-20 to identify the material model. The string *Shock* designates that the equation-of-state will be determined from the Shock EOS model. The three real-number parameters are C_0 (m/s), S_1 and S_2 (s/m).

MATERIAL MatNo GAMMA Gamma
MATERIAL 3 GAMMA 2.53

Defines material *MatNo* as an gamma-law material where pressure p is related to internal energy U by Eq. 18. The initial density and internal energy of the material in a particular region can be set with the *Region* commands of Sect. 6.10. The parameter *MatNo* is an integer in the range 1-20 to identify the material model. The string *Gamma* designates that the equation-of-state will be determined from the gamma-law model The real number parameter is the γ value.

MATERIAL MatNo VOID [DV PV]
MATERIAL 6 VOID 0.005 90.0E9

Void regions are placed between initially separated material regions. They provide logical continuity of the finite-element mesh. A void region must consist of a single element. The void has no effect on the hydrodynamic problem when its width exceeds the quantity W_v. The pressure rises if the width drops below W_v according to the Eq. 50. The optional real-number parameters D_v (in meters) and P_v (in pascals) is associated with material number *MatNo*. Pick a value for P_v equal to the highest pressure expected in the region. If values is are not specified, d_V is set equal to the width of the smallest element in the simulation space and $p_V = 100.0$ GPa.

6.8 Explosive material properties

This section covers the form of the *Material* command that defines the **KB** parametric model for explosives (discussed in Sect. 2.3). A typical simulation starts with the creation of a shock wave in the explosive by an initiator. The shock could be produced by collisions between regions, a rapid local heating, or the influence of an adjacent explosive. During the ignition phase it is sufficient to treat the solid explosive with the shock EOS model. If the shock pressure in an element exceeds a minimum value, p_{init}, the element material undergoes a rapid chemical change. The simplifying assumption in **KB** is that the internal energy of the element instantaneously increases by Q (the specific heat of explosion) and that the material changes to a gaseous state. The detonation products are described by an ideal gamma-law equation-of-state. Although the model is relatively simple, is has two advantages: 1) the required material data are generally available and 2) the results are in good agreement with theoretical and experimental values for detonation front velocities.

Note that results are not sensitive to the exact choice of the shock EOS parameters C_0, S_1 and S_2. If you do not have values for a specific material or initial density, you can usually get satisfactory results with parameters of a material with similar properties. The quantity p_{init} should not be considered as an absolute property of an explosive, but rather a parameter that may be adjusted to model different types of behavior. Values just below the Chapman-Joguet pressure give well-defined detonation fronts. Lower values correspond to more sensitive explosives, such as inhomogeneous materials with potential hot spots.

MATERIAL MatNo EXPL C0 S1 S2 PInit Q Gamma [INIT]
MATERIAL 5 EXPL 2461.0 3.517 -8.810E-04 2.0E10 5.183E+06 2.63

The initial density and internal energy of the material in a particular region may be set with *Region* commands of Sect. 6.10. The parameter *MatNo* is an integer in the range 1-20 to identify the material model. The string *Expl* designates that the equation-of-state will be determined from the explosives model. There are six real-number parameters. The quantities C_0 (m/s), S_1 and S_2 (s/m) define the shock equation-of-state for the undetonated material. The quantity p_{init} (Pa) is a threshold pressure for detonation, The quantity Q (J/kg) is the specific energy released in the explosion, and γ defines the equation-of-state for the gaseous detonation products. If the string parameter *Init* is included, the material will detonate at $t = 0.0$. This option is useful for checking the safety of explosive configurations. Self-ignited material should not cause a detonation wave.

6.9 Defining the system geometry

Defining geometry in a one-dimensional simulation is easy. **KB1** requires only a single command. Depending on the setting of the *Geometry* command, the simulation volume can have three different forms:KB1!symmetry types

RECT: a slab of material between the limits x_{min} and x_{max} with infinite extent in y and z.

CYLIN: a cylindrical shell of material between limits r_{min} and r_{max} with infinite extent in z. Note that **KB1** can handle a solid cylinder with $r_{min} = 0.0$.

SPHERE: a spherically symmetric shell of material between the limits r_{min} and r_{max}. Note that **KB1** can handle a solid sphere with $r_{min} = 0.0$.

The solution volume is divided into *regions* where elements have like properties. For example, the elements in two adjacent regions may consist of different materials. Another possibility is that the consist of the same material but have different initial conditions, such as directed velocity or density. You may also vary the element size by dividing a material volume into several regions. For example, to model a converging cylindrical shock it is often necessary to use smaller elements near the axis to preserve accuracy. There are two rules for defining a geometry in **KB1**:

Regions must be defined in order from left to right (x_{min} to x_{max}) in planar simulations. In cylindrical or spherical systems, regions must be defined from inside to outside ((r_{min} to r_{max}).

The regions must fill the space between x_{min} and x_{max} or r_{min} and r_{max}/ Any initially empty spaces must be filled with single-element voids.

The following command sets the properties of regions:

REGION RegNo MatNo Ri Ro NElem
REGION 5 1 0.000 0.002 50
KB1 script commands!RegionThe integer quantity *RegNo* is the region number (maximum value 127). Regions must be numbered sequentially $RegNo = 1$ as they appear in the file. The integer parameter *MatNo* is the number of the material model associated with the region. The code issues an error message if a material number has not been defined. The two real-number parameters *Ri* and *Ro* are the left and right (or inner and outer) boundaries of the region. Enter the dimensions in meters. Finally the integer number *NElem* is the number of uniform-width elements in the region.

The following illustrates a valid geometry definition for a cylindrical shell:

```
REGION 1 1 0.005 0.010 20\\
REGION 2 1 0.010 0.050 20\\
REGION 3 2 0.050 0.150 50
```

Note that the region numbers are in order and that the spatial dimensions proceed from left (inside) to right (outside). The start radius of a region equals the end radius of the previous region. Regions 1 and 2 consist of the same material, but the elements in Region 1 are smaller. Region 3 consists of a different material. **KB1** uses dynamic memory allocation, so the total number of elements is limited only by the installed memory of the computer.

6.10 Setting region properties

You can set initial properties of individual regions with the following commands.

VELINIT RegNo VInit [WEIGHTED]
VELINIT 5 10.0E3
The default initial region velocity is zero. The optional string *Weighted* applies only to cylindrical and spherical geometries. If it does not appear, all elements in the region have the same initial velocity. In this case, the relative size of elements in a cylindrical or spherical compression changes more rapidly on the inside of a layer and the density becomes non-uniform. When the *Weighted* option appears, the element velocity is assigned as $v_e(r) = v_{init} r_i / r$ for cylindrical systems or $v_e(r) = v_{init} r_i^2 / r^2$ in spherical geometries. The scaling ensures uniform density for converging or diverging shells. Note that the velocity *VInit* occurs at the inside of the region. The integer parameter *RegNo* is the region number. The real-number parameter *VInit* is the initial velocity in m/s. The string parameter *Weighted* is optional.

HYDINIT RegNo Rho Temperature
HYDINIT 4 1753.0 298.0
This form of the *HydInit* command applies to **KB** table materials. You can check the validity of the initial internal energy and pressure interpolations by checking the list in the `KLS` file. The *HydInit* command has no effect on a *Void* material. The integer parameter *RegNo* is the region number. The two real-number parameters are the initial density (in kg/m^3) and temperature (in ^{o}K).

HYDINIT RegNo Rho U
HYDINIT 6 860.0 0.0
This form of the *HydInit* command applies to *Gamma*, *ShockEOS* and *Explosive* materials. The *HydInit* command has no effect on a *Void* material. The integer parameter *RegNo* is the region number. The two real-number parameters are the initial density (in kg/m^3) and internal energy (in J/kg). Normally the internal energy equals zero.

VISCOSITY RegNo Viscosity
VISCOSITY 5 10.0
In hydrodynamic shock simulations, it is essential to include artificial viscosity forces to damp short-wavelength disturbances. You can assign relative viscosity terms individually to each region. If the value is too low spurious oscillations will occur near the shock front. If the value is too high the shock will spread in space. Ideally, the change in properties across the shock should extend over a few elements. The integer parameter *RegNo* is the region number. The parameter *Viscosity* is a dimensionless real number. The default value is *Viscosity* = 5.0.

HEAT RegNo TabName [TMult, PowMult]
HEAT 5 PulseFunc 35.0E-6 4.2E6
With this command, you can specify time-dependent addition of internal energy to the elements

of a region. The feature facilitates modeling of pulsed energy deposition by electric discharges, laser light or microwave radiation. The integer parameter *RegNo* is the region number. The string parameter *TabName* is the full name of a waveform table. The table specifies the temporal variation of the rate-of-change of internal energy. The preparation of tables was discussed in Sect. 6.6. Each data line contains the following two entries

```
t (seconds)    du/dt (J/kg-s)
```

The optional parameters *TMult* and *PowMult* are multiplication factors that modify values of t and $\mathrm{d}u/\mathrm{d}t$ as they are entered in the program. The time integral of $\mathrm{d}u/\mathrm{d}t$ over the span of the table gives the total internal energy added to (or subtracted from) the elements of the region.

6.11 Diagnostics

The commands of this section control the data files created by **KB1.** There are two types of information available from an initial-value simulations: 1) records of quantities over the full solution volume at specified times (spatial data dumps) and 2) records of quantities at all time steps at specified positions (probes). Three commands control the creation of spatial dumps.

DIAGDT DTime
DIAGDT 5.0E-6
Write a data dump at approximately uniform time intervals. Because the time step may vary, the record may not occur at an exactly uniform interval. The convention is that **KB1** writes the spatial information at or immediately after the specified time. The real-number parameter *DTime* is the time interval in seconds.

DIAGTIME TDiag
DIAGTIME 7.333E-8
You can set up to 50 specific times to make data dumps. For example, you may want to create a detailed set of views at the collision time of two regions. This command can work in conjunction with the *DiagDt* command. The data dump occurs at or immediately after the specified time. The *DiagTime* commands must appear in the input script in chronological order (*i.e.*, ordered from the earliest to the latest data dump). Enter the time *TDiag* in seconds.

DIAGSTEP NDiag
DIAGSTEP 200
When this command is issued, **KB1** makes a data at intervals separated by a given number of time steps. This command works in conjuction with the *DiagDt* and *DiagTime* commands. Be careful entering dump information, or you may fill a hard disk with data. The integer parameter *NDiag* is the number of time steps between data dumps.

The final two commands control the placement of probes in the solution volume. **KB1** can create from 1 to 12 probe files with names of the form `RunName.P01`, `RunName.P02`,.... Information in the files may be plotted or analyzed with the **Probe** program (Chap. 10).

SETPROBE NPElem
SETPROBE 58

Probes are located at the center of an element. The output files contain the corresonding element quantities (density, pressure, ...). Node quantities (position, velocity) are calculated at the element center-of-mass. The integer parameter *NElem* is number of the element where the probe should be located.

PROBESTEP NStepProbe
PROBESTEP 5

Simulations with short time step may run for thousands of time steps. In this case, there is no need to record probe information at each step because only 200-300 points are sufficient for a good plot. he purpose of the *ProbeStep* command is to keep probe files at a manageable length. The command instructs **KB1** to make entries in probe files at intervals. For example, if $NStepProbe = 5$ the code makes a record every fifth time step. T The default value is $NStepProbe = 1$.

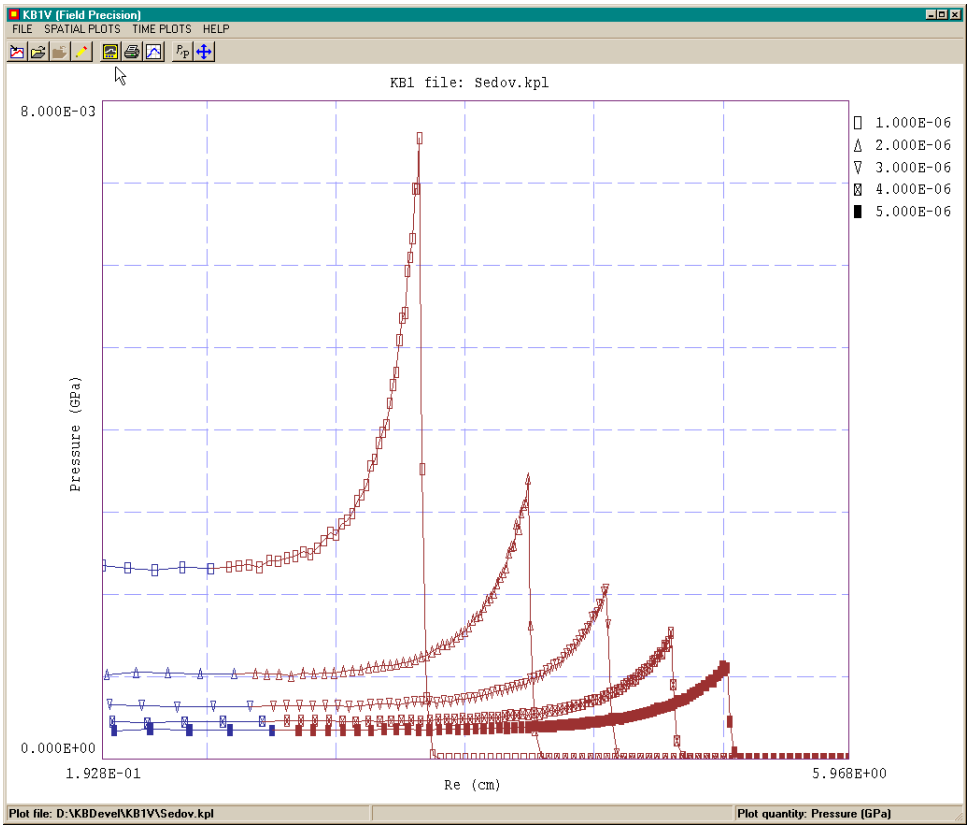

Figure 18: **KB1V** screen showing a spatial plot.

7 KB1V

KB1V is an analysis program for output from **KB1** (one-dimensional hydrodynamic solutions). **KB1V** makes screen and hardcopy plots of data stored in the binary **KB1** plot files (`FPrefix.KPL`). The program creates plots in linear or log format with automatic scaling and grids. **KB1V** features a digital oscilloscope mode for active inspection of data. Quantitative information from an analysis session may be recorded in a data file. You can run `kb1v.exe` directly or from the **KB** program launcher.

7.1 File menu

Figure 18 shows the **KB1V** screen display. The program window has has popup menus and a toolbar at the top and a status bar at the bottom. When the program starts only the *File* and *Help* menus are active. The plotting functions become active after a data file is loaded. The *File* menu contains the following commands:

LOAD PLOT FILE

This command displays a dialog to load a plot file (`FPrefix.KPL`) into the program. You can change the current working directory from within the dialog. Only one file MAY be loaded at a time. The plot file contains information on hydrodynamic quantities in all elements at times

specified by the **KB1** *NDiag*, *MakeDiag* and *DTime* commands. The *Spatial plot* and *Time plot* menus become active after the file is loaded.

OPEN DATA FILE

When a data file is opened **KB1V** records the values used to create plots. The program also records point data in the oscilloscope mode. The resulting text file may be edited or imported into a spreadsheet.

CLOSE DATA

This command terminates file listings and closes the current data file. Be sure to close a data file before you attempt to *Edit* it or use it in another program.

EDIT FILE

This command brings up a dialog to pick a file, and then opens it in a full-featured Windows text editor. Changing directories in the dialog does not change the working directory of the program.

7.2 Spatial plot menu

Spatial plots show the spatial distribution of a chosen hydrodynamic quantity over all elements (*i.e.*, a **KB1** data dump). As shown in Fig. 18, information from multiple data dumps may be superimposed. Each curve has optional plot symbols that designate the dump and show the center-of-mass locations of the elements. The time corresponding to each plot is shown in the legend on the right. Lines and plot symbols are color-coded by either the region number or material number of the corresponding element.

SCREEN PLOT

This command initiates a spatial plot or refreshes the screen.

HARDCOPY PLOT

Redirects the current screen plot to the Windows **Default** printer. If you have multiple printers, be sure to set the desired device as the default using *Settings/Printers* before initiating the plot.

PLOT FILE (EPS)

Redirects the current screen plot to a plot file in Encapsulated PostScript format in the current directory. The program prompts for a file prefix and creates a file with a name of the form `FPrefix.EPS`.

PLOT FILE (BMP)

Redirects the current screen plot to a plot file in Windows Bitmap format in the current directory. The program prompts for a file prefix and creates a file with a name of the form `FPrefix.BMP`.

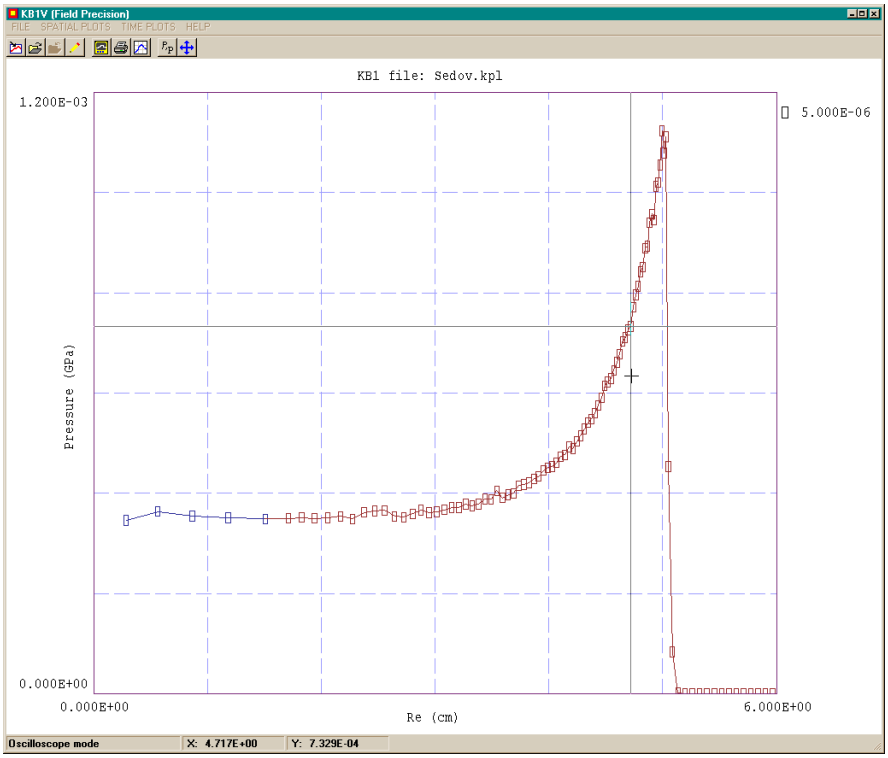

Figure 19: Operation in the oscilloscope mode.

OSCILLOSCOPE

This command is active when a screen plot has been displayed. In the oscilloscope mode (Fig. 19, the program displays a cross-hair pattern that you can drag with the mouse. The x and y coordinates of the current point are displayed in the status bar. If a listing file is open, press the left mouse button to record a point in the file. All other menu functions are deactivated in the oscilloscope mode. Press the right mouse button or *ESC* key to return to normal program operation. Note that when multiple plots are displayed on the screen, the oscilloscope function uses the last plot drawn.

SET INCLUDED PLOTS

The program displays a dialog (Fig. 20) that lists the times of all data dumps recorded in the KPL file. Use the left mouse button to highlight any number of dumps to plot. Resetting the highlight removes the associated plot.

SET PLOT QUANTITY

Choose the hydrodynamic quantity to be plotted. Note that a choice of the quantity element position r_e) in a spatial plot produces a straight line with unity slope. The quantity is included for *Time plots*.

SET PLOT LIMITS

Displays a dialog (Fig. 21) to set the horizontal or vertical plot limits manually or to restore

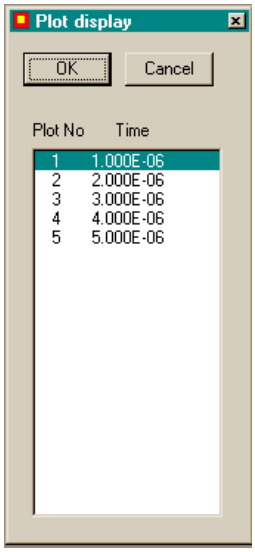

Figure 20: Plot display dialog

autoscaling. In the autoscaling mode, the program searches all plotted data dumps to find limits so that the display fills the screen and all data points are included. If you change the plotted quantity, it may be necessary to restore autoscaling to make the plot visible on the screen.

SET LOG/LIN

KB1V can display quantities on the horizontal or vertical axis in linear or log format. Note that negative values are omitted from log plots.

SET MAT/REG

In spatial plots the symbols are color-coded according to the identity of the element. This feature makes it easy to see the behavior of material boundaries. The color can be assigned according to the material or region number of the element.

TOGGLE SYMBOLS

Turn plotting symbols on or off. The symbol shape denotes the data dump in multiple plots. The symbol color corresponds to either the region or material number.

TOGGLE GRID

Turn plot grid lines on or off. The line spacings are automatically set to easily recognized intervals along linear axes (*i.e.*, 0.002, 0.005, 0.010, ...).

PLOT FILE INFORMATION

Displays information about the plot file (*i.e.*, number of elements per plot, number of plots,...).

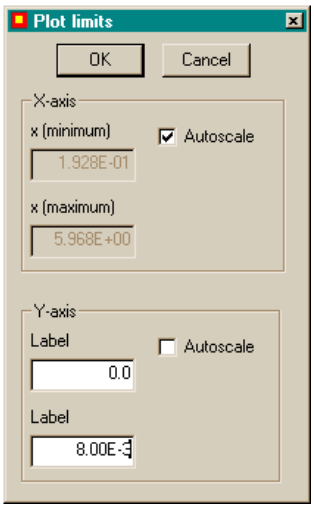

Figure 21: Plot limit dialog.

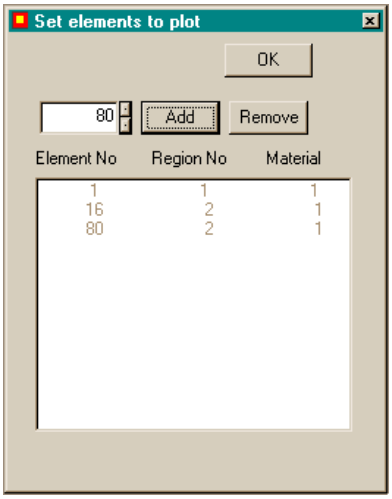

Figure 22: Set included elements dialog.

7.3 Time plot menu

If a plot file contains a large number of data dumps, you can create useful plots of hydrodynamic quantities as a function of time for any elements. With one exception, the commands serve the same functions as those in the *Spatial plot* menu.

SET INCLUDED ELEMENTS

The program displays a dialog (Fig. 22) where you can add or subtract elements (identified by index number) from the plots. Set the target element number using the spinner at the top left and then click a button to add or remove the element from the list. The listing box shows the material number and region number of displayed elements.

The `Help menu` contains a single command:

KB MANUAL

Display this document. The file kb.pdf must be in the same directory as kb1v.exe.

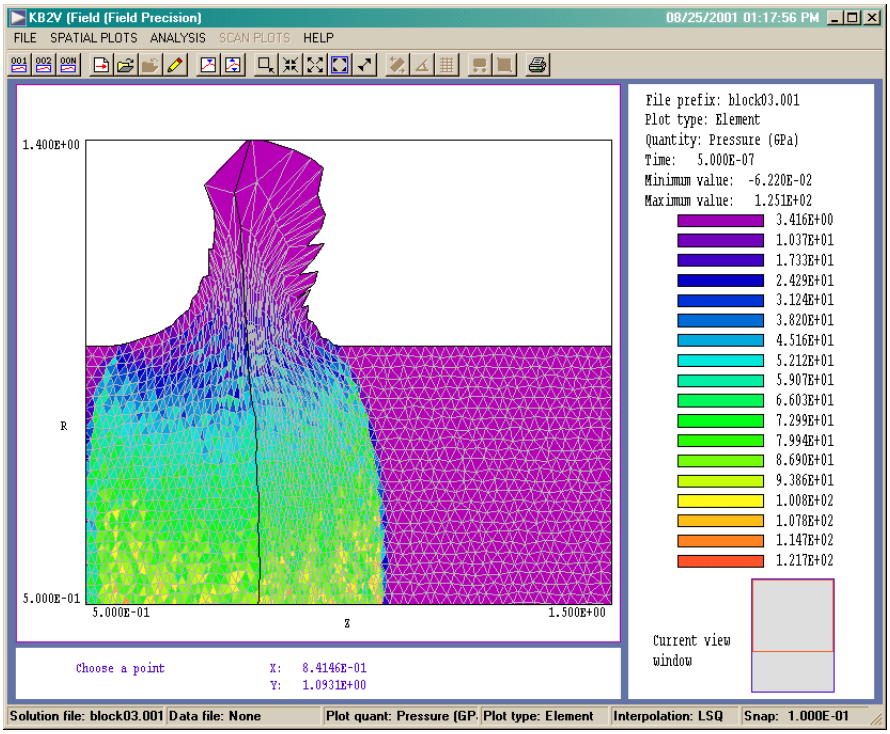

Figure 23: **KB2V** postprocessor – screen shot for example `BLOCK03`.

8 KB2

8.1 Introduction

KB2 is a versatile software system for simulations of shock hydrodynamics. The program handles two-dimensional cylindrical or planar geometries through a unique finite-element method that is well-suited to systems that undergo large changes in volume. This manual covers procedures to set up **KB2** runs. The program employs the **Mesh** program, the standard mesh generator for the Field Precision **TriComp** series of two-dimensional finite-element codes. Once the mesh for the initial system geometry is created, the commands to control **KB2** runs are straightforward. The mathematical foundation of the code is described in Chap. 2 The software package employs the following programs:

Mesh: versatile utility to create conformal triangular meshes from user-specified geometries.

KB2: main simulation program controlled by an input script.

KB2V: interactive graphical post-processor for data files (spatial variations of quantities at specified times)

Probe: plotting and oscilloscope utility, used to inspect and to plot **KB2** probe files.

Probe is described in Chap. 10. Table 9 summarizes physical units used in **KB2** and **KB2V**.

Table 9: Physical units for the **KB2** programs

Quantity	**KB2**: internal operations, data and history files	**KB2V** and **Probe**
Density	kg/m^3	gm/cm^3
Position	m	Set by *DUnit*
Pressure	Pa	GPa
Temperature	^oK	^oK
Internal energy	J/kg	MJ/kg
Velocity	m/s	km/s

The following section summarizes the organization of **KB2** runs. A detailed description of an example is included to familiarize you with the format of input data and the relationship of components in the software system. The two required input files are:

an output file from Mesh describing the initial geometry of the system, and

a **KB2** script that provides physical information for the simulation.

Section 8.3 covers special techniques used in **Mesh** to create conformal triangular meshes for hydrodynamic simulations. The material supplements the **Mesh** manual. Section 8.4 covers the structure and syntax conventions of the **KB2** control script. The section covers methods to define applied pressure waveforms. Pressures applied on the system boundaries is one method to initiate shock hydrodynamic processes in **KB2.** The other two methods are:

assignment of initial velocities to regions of the solution space, and

detonation of explosive materials.

8.2 Running KB2

As an introduction we shall walk through the steps of a hydrodynamic solution. It is assumed that the executable files It is assumed that the files `RT_INSTAB.MIN`, `RT_INSTAB.KIN`, `ALUM3715.KBT` and `STEPFUNC.DRV` are available in a working directory. To begin, set the Data directory the KB program launcher.

Figure 24 shows the initial simulation geometry for the `RT_INSTAB` example. A 1 mm thick aluminum plate is accelerated by a zero-mass fluid on the right-hand side with peak pressure 5 GPa. The applied pressure follows a step-function variation with a risetime of 0.1 μs. The plate surface has an initial perturbation on the upstream side such that the plate thickness varies from 1.00 mm to 1.05 mm. The sinusoidal variation has a wavelength of 2.5 mm in the vertical direction. The simulation represents 10 mm of a plate that extends infinitely in the vertical direction. Special symmetry boundaries are defined at the top and bottom. Figure 24 shows a portion of the plate along with the outlines of mesh elements from $y = 0.0$ to 2.0 mm.

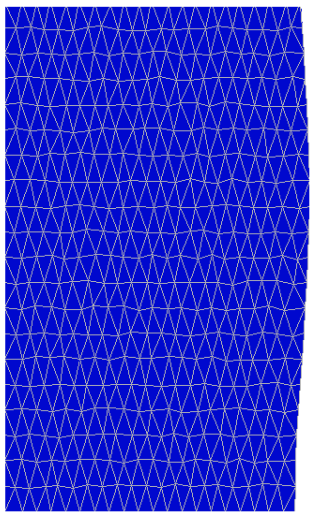

Figure 24: Mesh for the initial geometry of the example `RT_INSTAB`.

Run **Mesh** by clicking on the entry of the **KB** program launcher. Click on the *Load script (MIN)* command of the *File* menu. If all files are in the correct location, the choice in the dialog should include `RT_INSTAB.MIN`. Pick the file and click *OK*. Next, click on the *Process* command. The program analyzes specifications in the script to set up the geometry of Fig. 24. Click a mouse button to proceed. Finally, pick the command *Save file (MOU)* in the *File* menu. At this point, you have created the file `RT_INSTAB.MOU`, one of the required inputs for the **KB2** run. At this point you can experiment with some of the plotting capabilities of **Mesh**.

Before leaving the **Mesh** program, it is useful to inspect the input script `RT_INSTAB.MIN`. In the *File* menu, click on the command *Edit current script (MIN)*. A shortened version of the file is shown in Table tab:rtinstabmin. Two lines in the *GLOBAL* section are of interest

```
TriType Glass 0.10\\
Smooth 0
```

In the *Glass* option of *TriType*, the program introduces random node displacements in the initial logical mesh to create the disordered set of elements of Fig. 24. The *Smooth 0* command turns off the mesh smoothing that normally occurs after boundary fitting operations. This operation would wash out the initial perturbations. Disordered initial meshes are usually preferable for hydrodynamic simulations. Numerical errors can accumulate when mesh boundaries are lined up, resulting in a spurious shear plane.

The geometric sections describe six regions. Region 1 is a *Filled* region that represents the aluminum plate. Most of the specification lines define the irregular upstream boundary. After setting the boundaries, **Mesh** labels all nodes and enclosed elements as $RegNo = 1$ (blue triangles in Fig. 3). The remaining *Open* regions set the properties of nodes on the boundary of the solution volume. The top and bottom boundaries are *Sliding* surfaces that can move only in the direction of the unit vector (1.0,0.0). This condition is useful to represent symmetry boundaries. The nodes on the right-hand side of the solution-volume are *Pressure* points. They respond as though any adjacent elements outside the solution volume had an applied pressure.

Be sure you have saved the mesh by checking the status bar, and then exit **Mesh**. Next, run **KB2.** The commands and operational options are identical to those of KB1 (Sect. 6.2)

Table 10: Mesh input file RT_INSTAB.MIN

```
GLOBAL
   XMesh
     0.00  1.10  0.05
       End
   YMesh
     0.00 10.00  0.100
       End
   TriType Glass 0.10
   Smooth 0
END
REGION  FILL   1
* Aluminum flyer plate
     L  0.00  0.00  1.00  0.00
    L    1.00000   0.00000   1.00079   0.10000
    L    1.00079   0.10000   1.00309   0.20000
   ...
    L    1.00309   9.80000   1.00079   9.90000
    L    1.00079   9.90000   1.00000  10.00000
     L  1.00 10.00  0.00 10.00
     L  0.00 10.00  0.00  0.00
   END
REGION   2
* Slide boundary: top
     L  0.00  10.00  1.00  10.00
   END
REGION   3
* Slide boundary: bottom
     L  0.00   0.00  1.00   0.00
   END
REGION   4
* Pressure boundary: right-hand side
    L    1.00000   0.00000   1.00079   0.10000
    L    1.00079   0.10000   1.00309   0.20000
   ...
    L    1.00309   9.80000   1.00079   9.90000
    L    1.00079   9.90000   1.00000  10.00000
   END
REGION   5
* Pressure and slide point: top
     P  1.00  10.00
   END
REGION   6
* Pressure and slide point: bottom
     P  1.00   0.00
   END
ENDFILE
```

Table 11: KB2 input file RT_INSTAB.KIN

```
*  RT\_INSTAB.KIN
* ------------------ Run control --------------------
  Geometry: Planar
  Dt: 1.0E-9
  TMax: 2.501E-6
  DUnit: 1000.0
  Interporder Second
  Pressure 1 StepFunc.DRV 0.10E-6 5.0E9
* -------------- Material properties ----------------
  Material 1 KBT ALUM3715
* --------------- Region properties -----------------
  Region 1 Material 1
  Viscosity 1 10.0
  Region 2 Sliding  1.0  0.0
  Region 2 Material 1
  Region 3 Sliding  1.0  0.0
  Region 3 Material 1
  Region 4 Pressure 1
  Region 4 Material 1
  Region 5 Pressure 1
  Region 5 Sliding  1.0  0.0
  Region 5 Material 1
  Region 6 Pressure 1
  Region 6 Sliding  1.0  0.0
  Region 6 Material 1
* ------------------ Diagnostics --------------------
  DiagTime 0.0
  DiagDt 0.5E-6
* Probes at minimum and maximum plate thickness
  SetProbe 1.016 1.200
  SetProbe 0.945 2.500
  ProbeStep 20
* ------------------------------------------------
  EndFile
```

Click on the command *Edit input files* on the *File* menu and pick the file RT_INSTAB.KIN. This file, the control script for **KB2**, is listed in Table 11. The commands of the control group set a maximum run time of 2.5 μs and specify that the coordinates from **Mesh** should be converted from millimeters. The *Pressure* command loads and modifies a set of numbers from the data file StepFunc.DRV to define a step-function applied pressure that rises from 0.0 to 5.0 GPa in 0.1 μs. The *Material* command loads the equation-of-state table ALUM3715.KBT as $MatNo = 1$. The *Region* commands set properties of the mesh regions and associate all of them with material $MatNo = 1$.

Exit the editor and click the *Run* command. Pick the file RT_INSTAB.KIN in the dialog. The program initiates the run and reports progress in the screen window. The run time will depend on the speed of your computer and should be a few minutes. After the run is completed, you can use Windows Explorer or your file manager to confirm that the program has created the following output files:

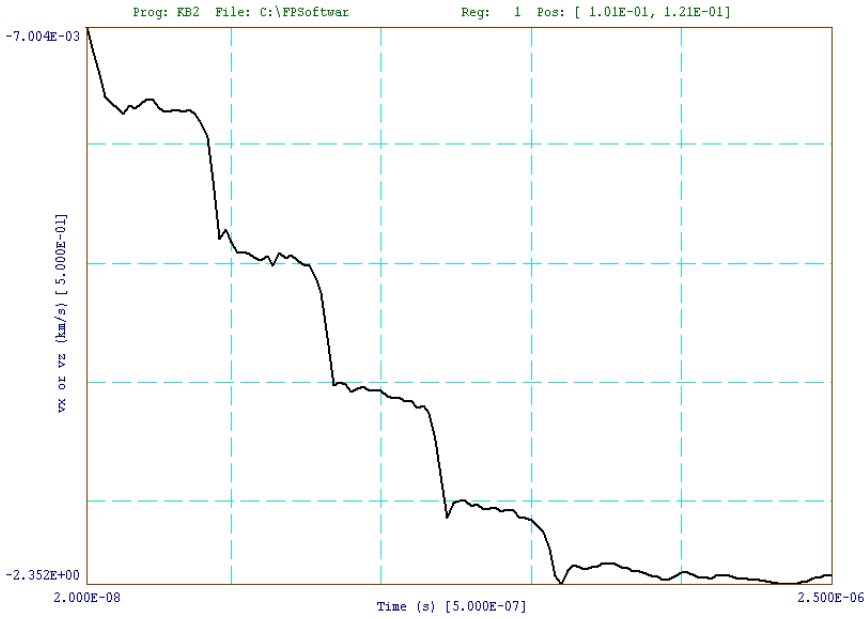

Figure 25: Plot created by **Probe** for the RT_INSTAB example.

```
RT_INSTAB.KLS
RT_INSTAB.001, ..., RT_INSTAB.006
RT_INSTAB.P01
RT_INSTAB.P02
```

The file RT_INSTAB.KLS is a listing of run information that is often useful for debugging. The six files with numbered suffixes are data dumps at times 0.0, 0.5,...,2.5 μs. The two files RT_INSTAB.P01 and RT_INSTAB.P02 are probe records at the two positions defined by the *Set-Probe* commands.

The **Probe** program (Chap. 10)is a utility to plot information recorded in probe files. The program is described in a separate manual. Run the program and click on the command *Load probe file*. Pick the file RT_INSTAB.P01. Under *Plot parameters* choose the command *Set plotted quantity*. Pick the quantity v_x to display the plot of Fig. 25. It shows a general acceleration of the aluminum plate to about 2.3 km/s. The effect of shock reflections through the plate is apparent. The final step is to analyze the data dumps with the **KB2V** postprocessor (Fig. 23). Run the program and pick the command *Load first solution file* from the *File* menu. Choose RT_INSTAB.001 and click *OK*. The program loads the first data file created at t = 0.0 μs before the application of the applied pressure. Click on *Plot type* in the *Spatial plot* menu and choose the *Region* option. Next, click on *Toggle element outline* in the *Spatial plot* menu. Using the *Zoom* and *Pan* functions you should be able to inspect the initial mesh and recreate the plot of Fig. 25.

Reset the plot type to *Element* and click on *Load next solution file* in the *File* menu. This loads the data dump created at 0.5 μs. Click on *Plotted quantity* in the *Spatial plot* menu and choose *Density*. The program displays the plot of Fig. 26 which shows a compression wave created by the pulsed pressure moving through the plate. At this point, you can experiment with the plot and analysis capabilities of **KB2V**. Chapter 9 describes the program in detail. Figure 27 shows a plot constructed from the results of the RT_INSTAB example. The spatial

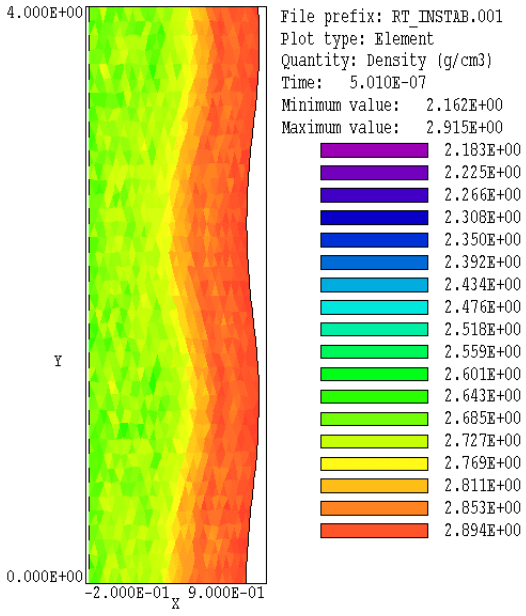

Figure 26: Density profiles at 0.5 μs, `RT_INSTAB` example.

limits of the pressure plots at 0.5 and 2.5 μs have been adjusted to display the data in real space (Eulerian view). The plate accelerates to the left. The pressure boundary condition is equivalent to acceleration by a zero-mass fluid. In this case, the upstream boundary is subject to the Rayleigh-Taylor instability. The example illustrates the capability of **KB2** to follow the instability well into the non-linear regime.

8.3 Mesh generation techniques

The **Mesh** program is used to define element divisions that represent the initial state of a physical system. The success of **KB2** solutions may depend on details of the initial mesh. **Mesh** script commands have been added to help in the creation of logical meshes for hydrodynamics. The first controls the general shape of elements.

TRITYPE [TriType] [RandDisp]
TRITYPE GLASS 0.15

This command sets the general shape of triangular elements. The string *ISO* denotes the standard row-oriented isosceles triangles that are generated by default (Fig. 28*a*). In response to the string *RIGHT,* Mesh fills the logical mesh region with right-angle triangles ((Fig. 28*b*)). The string *GLASS* gives an irregular mesh. Here, random displacements are added at nodes to randomize the element sizes and shapes ((Fig. 28*c*)). This option can help remove interference effects resulting from coherent element motion parallel to the sides of a regular element array. An optional real-number parameter *RandDisp* may be added to the *GLASS* option to control the size of the displacements. Values in the range 0.05 to 0.25 are useful. The default is $RandDisp = 0.10$.

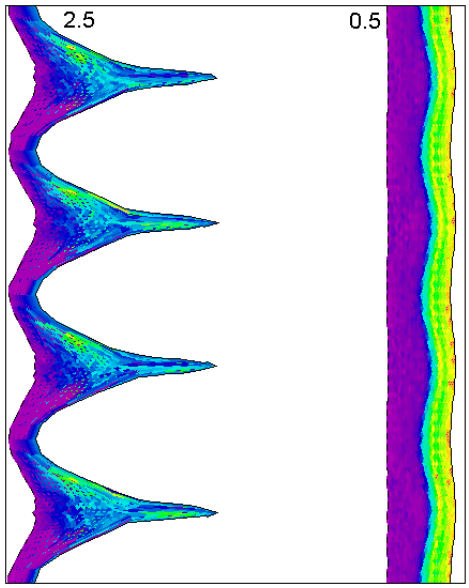

Figure 27: Outline of a 1 mm aluminum plate accelerated by a zero-mass fluid at 5 GPa. Abscissa: $x_{min} = -6.0$ mm, $x_{max} = 1.0$ mm. Ordinate: $y_min = 0.0$ mm, $y_{max} = 10.0$ mm.

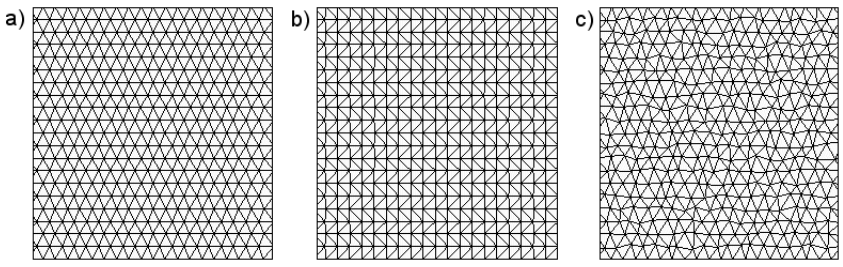

Figure 28: Logical mesh types: *a*) ISO, *b*) *RIGHT*, *c*) *GLASS*.

SMOOTH NSmooth
SMOOTH 0
This command deactivates node smoothing after boundary fitting. It must be included when the *GLASS* triangle type is used. Otherwise, the final mesh will be smoothed to a set of isosceles triangles.

TRANSFORM TransType
TRANSFORM CYLIN
This command maps one logical mesh onto another. Presently, the only option for the string *TransType* is *CYLIN*.

A transformed mesh may be useful to represent the cross-section of an initially cylindrical object in planar geometry or a spherical shell in cylindrical geometry. The x axis coordinates on the original logical mesh are interpreted as radii and the y axis coordinates are interpreted as angles (in degrees). The transformed coordinates are:

$$\begin{aligned} x' &= x\cos(y), \\ y' &= x\sin(y). \end{aligned} \tag{51}$$

Figure 29 shows the logical mesh generated by the following commands:

```
Transform Cylin
XMesh
   2.00   5.00   0.10
End
YMesh
  -30.0   30.0   2.0
End
```

8.4 Script commands

KB2 may use and create several types of files. Table 12 summarizes the function of different files. At files are in text format. In this section, we shall concentrate on the preparation of the input script, the fundamental control file required for all **KB2** runs. The format and syntax conventions are similar to those of the **KB1** script (Sect. 6.4). The file must have a name of the form `FPrefix.KIN`, where *FPrefix* is a valid filename from 1 to 46 characters in length. The script and other input files for mesh geometry, equation-of-state data and pressure waveforms should be in the same directory.

Command groups are the same as those for **KB1** (Sect. 6.4). Some commands have the same function and format as those in **KB1**, while others take a different form to support the two-dimensional geometry. This section emphasizes similarities and differences in the command sets. The following control commands are identical to those in **KB1** (Sect. 6.5):

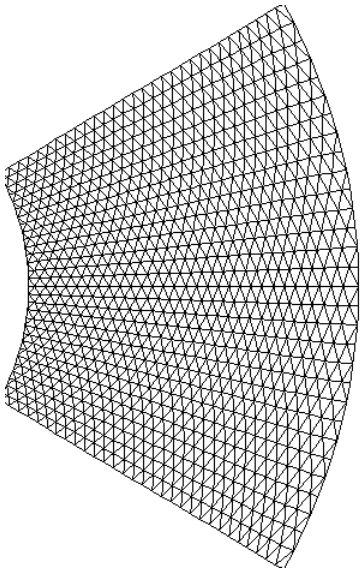

Figure 29: Logical mesh generated with the *Transform* command.

Table 12: **KB2** input and output files

Name form	**Function**
`FPrefix.MIN`	Input file for the Mesh program, description of the initial system geometry
`FPrefix.MLS`	Listing of information and error messages from Mesh
`FPrefix.MOU`	Mesh specification file created by Mesh, required input for KB2
`FPrefix.KIN`	Required input script controls operation of KB2
`PressName`	Input table of waveform values for an applied pressure
`KBTName.KBT`	Input equation-of-state table for a KBT material
`FPrefix.KLS`	KB2 output listing file with extensive run information and data
`FPrefix.O01`	KB2 output data dumps for **KB2V** analyses
`FPrefix.P01`	Files of temporal information for a given element for Probe analyses
`GPrefix.DAT`	Data file created during a **KB2V** analysis session

TMAX TMax
TITLE Run title string
SAFETY Safety
NCHECK NCheck
DT Dt
DTCHANGE TChange DtNew
INTERPORDER [First, Second]
ERRSTATUS [All,Partial,None]

The definition of pressure waveforms is described in Sect. 6.6. In **KB2**, specified time-dependent pressures are not limited to the inner and outer nodes of the solution volume. They may be applied to the nodes of line regions of any shape. Therefore, the pressure definition commands have slightly different forms:

PRESSURE TabNo TabName
PRESSURE 3 LinDrive.PRS
Up to five *Pressure* commands may appear in the input script to define applied pressure waveforms that may be applied on different boundary regions. The quantity *TabNo* is a reference number for the table (an integer in the range 1-5). The string parameter gives the full name of a tabular function file in the current data directory.

PRESSURE TabNo TabName TMult PMult
PRESSURE 3 LinDrive.PRS 1.0E-06 25.0E09
With this form of the *Pressure* command, time values are multiplied by *TMult* and pressure values by *PMult* when they are loaded into the program. This feature makes it convenient to maintain a library of normalized waveforms, using multiplication factors to apply them to different simulations. The quantity *TabNo* is a reference number for the table, an integer in the range 1-5. The string parameter gives the full name of a tabular function file in the current data directory.

Commands to set material properties are the same as those in **KB1** (Sects. 6.7 and 6.8):

MATERIAL MatNo KBT TabName
MATERIAL MatNo SHOCK C0 S1 S2
MATERIAL MatNo GAMMA Gamma

Because logical connectivity must be maintained in the triangular mesh, there is no equivalent of the *Void* material.

The system geometry is determined by an output file from the **Mesh** program. If the **KB2** script has the name `FPrefix.KIN`, the program will seek a mesh file with the name `FPrefix.MOU`. The following two commands specify how the geometry should be interpreted:

GEOMETRY [PLANAR, CYLINDRICAL]
GEOMETRY CYLINDRICAL
This required command sets the solution symmetry. **KB2** can perform calculations in planar geometry or cylindrical. In the first case, quantities may vary in the x-y plane and are uniform in z. In cylindrical geometry, quantities vary in z and r with azimuthally symmetry.

DUNIT DUnit
DUNIT 100.0
Set a conversion factor for coordinates in the **Mesh** input file. The quantity *DUnit* equals the number of **Mesh** units per meter. For example, if dimensions in the mesh file are in mm, set $DUnit = 1000.0$.

In general, commands to set region properties in KB2 differ from those of KB1, so we shall list the full set. To begin, the following commands set the properties of elements in regions with non-zero volume. Some of the commands may also apply to the nodes of both filled and open regions.

REGION 5 MATERIAL 3
REGION RegNo MATERIAL MatNo
This required command associates elements and nodes marked by region number *RegNo* with the properties of material number *MatNo*.

HYDINIT 3 4500.00 530.0
HYDINIT RegNo Rho Temperature
Although two regions may be associated with the same material model, they can be assigned different initial hydrodynamic conditions. This form of the command sets the initial density (kg/m^3) and temperature (^{o}K) for regions associated with **KB** table materials. The program attempts to set the pressure and internal energy by interpolations on the tables. You can check the values in the `KLS` file. If the program has trouble interpolating on the low end of the table, you can usually find acceptable parameters using **KBView** (Chap. 5. The initial conditions of all regions with non-zero volume must be defined.

HYDINIT 4 4500.0 0.0
HYDINIT RegNo Rho Epsi
Use this form of the command to set the initial density (kg/m3) and internal energy (J/kg) for regions associated with *Gamma*, *Shock* and *Expl* materials. The initial conditions of all regions with non-zero volume must be defined.

VISCOSITY 5 0.25
VISCOSITY RegNo CVis
This command defines a value of the artificial viscosity coefficient for elements with region number *RegNo*. The default value is 10.0. Assign higher values if there are spurious oscillations at shock fronts and low values if shock fronts spread over several elements.

HEAT RegNo TabName [TMult, PowMult]
HEAT 5 PulseFunc 35.0E-6 4.2E6

With this command, you can specify time-dependent addition of internal energy to the elements of a region. The feature facilitates modeling of pulsed energy deposition by electric discharges, laser light or microwave radiation. The integer parameter *RegNo* is the region number. The string parameter *TabName* is the full name of a waveform table. The table specifies the temporal variation of the rate-of-change of internal energy. The preparation of tables was discussed in Sect. 6.6. Each data line contains the following two entries

```
t (seconds)    du/dt (J/kg-s)
```

The optional parameters *TMult* and *PowMult* are multiplication factors that modify values of t and $\mathrm{d}u/\mathrm{d}t$ as they are entered in the program. The time integral of $\mathrm{d}u/\mathrm{d}t$ over the span of the table gives the total internal energy added to (or subtracted from) the elements of the region.

The remaining commands set the property of nodes. The *VelInit* command applies to both *Filled* (non-zero volume) or *Open* (line) regions. The other commands apply only to *Open* regions and are used to set boundary conditions.

VELINIT 3 Cart 0.000 -3.0E3
VELINIT RegNo CART vx vy

This command sets an initial velocity for all nodes associated with region *RegNo*. The string *CART* indicates that all nodes have the same velocity defined by [v_x,v_y] or [v_z,v_r]. Enter the velocity values in units of m/s.

VELINIT 3 RADIAL 0.000 0.000 -3.0E3
VELINIT RegNo RADIAL XConv YConv MagV

This command sets an initial velocity for all nodes associated with region *RegNo*. The string *RADIAL* indicates that nodes have velocities assigned to define a medium converging toward a point. The compression is cylindrical in *Planar* solutions, In *Cylindrical* solutions, the compression is spherical if the reference point is on the z axis. The quantities *XConv* and *YConv* define the convergence point (x,y) or (z,r). Enter the values in units set by *DUnit*. The quantity *MagV* is the magnitude of the velocity assigned to all nodes in units of m/s.

REGION 3 FIXED
REGION RegNo FIXED

This command assigns the *Fixed* (immovable) condition to nodes associated with region number *RegNo*. The condition is useful for symmetry boundaries and usually applies to line regions. A surface is immovable if 1) there are equal normal forces on both sides and 2) the tangential force is zero. The *Fixed* condition may also apply if a surface is adjacent to a material with infinite density.

REGION 7 SLIDING 0.7071 0.7071
REGION RegNo SLIDING ux uy

The *Sliding* boundary condition is useful for modeling symmetry boundaries in a periodic

system. Along such a boundary the normal force is zero but the tangential force may be non-zero. In response to such forces, the nodes can move only along the line defined by the unit vectors $[u_x,u_y]$ or $[u_z,u_r]$ in cylindrical problems). The condition applies only to line regions. The boundary should be a straight line aligned with the normal vector.

REGION 4 PRESSURE 2
REGION RegNo PRESSURE TabNo

This command sets nodes associated with region number *RegNo* as *Pressure* nodes and associates them with pressure table *TabNo* (see the *Pressure* command). Pressure regions must be line regions on the periphery of the solution volume. If a node has the *Pressure* attribute, **KB2** assigns the pressure from the associated table calculated at the current time to all adjacent elements with $NReg = 0$. In other words, the pressure is applied to elements (real or fictitious) outside the solution volume. In this way, time-varying pressures may be applied along boundary regions of arbitrary shape.

The example `RT_INSTAB` discussed in Sect. 12.5 is a good example of how to implement *Pressure* and *Sliding* boundaries. The following script file lines control the features:

```
01: Pressure 1 StepFunc.DRV 0.10E-6 5.0E9\\
02: Material 1 KBT ALUM3715

03: Region 1 Material 1\\
04: Viscosity 1 10.0

05: Region 2 Sliding  1.0  0.0\\
06: Region 2 Material 1

07: Region 3 Sliding  1.0  0.0\\
08: Region 3 Material 1

09: Region 4 Pressure 1\\
10: Region 4 Material 1

11: Region 5 Pressure 1
12: Region 5 Sliding  1.0  0.0\\
13: Region 5 Material 1

14: Region 6 Pressure 1\\
15: Region 6 Sliding  1.0  0.0\\
16: Region 6 Material 1
```

Line 1 loads data on the time variation of pressure from the normalized file `StepFunc.DRV`. The time values are multiplied by 0.10×10^6 to give a step-function risetime of 0.1 μs. The pressure values are multiplied by 5.0×10^9 to give a peak pressure of 5 GPa. The data are referenced as *Pressure Table* 1. Line 2 sets *Material Number* 1 as a *KBT* type and loads equation-of-state data. Line 3 associates *Region* 1 with *Material* 1, while Line 4 sets a value of artificial viscosity in the elements. Regions 2 and 3 are line regions at the top and bottom of the solution representing symmetry boundaries of the periodic system. They are free to move in

the x direction but cannot move in y. Lines 5 and 7 specify this condition. Note that there are also *Material* commands (Lines 6 and 8) for the region. They specify that the boundary nodes should be advanced like internal nodes surrounded by elements of *Material* 1 with corrections for the sliding condition. In the absence of these commands, the program would not advance the positions and velocities of the boundary nodes. Region 4 (Line 9) is the boundary on the right-hand side of the plate on which the pressure is applied. Note that a *Material* assignment command (Line 10) is included so that the node will be advanced in velocity and position. Regions 5 and 6 are single nodes at the top and bottom of the right-hand boundary. The special regions must be defined because the nodes, in contrast to those of Regions 2,3 or 4, must have both the *Sliding* and *Pressure* conditions.

The example `BLOCK03` illustrates how to set up *Sliding* boundaries for a solution with multiple materials with different initial velocities.

To conclude, the following diagnostic commands are the same as those in **KB1**:

DIAGDT DTime
DIAGTIME TDiag
DIAGSTEP NDiag
PROBESTEP NStepProbe

The following command has a different form in **KB2**:

SETPROBE XPos YPos
SETPROBE 0.50 5.67

Probes are located at the centers of elements. The output files list the corresponding element quantities (density, pressure, ...). Node quantities (position, velocity) are evaluated at the element center-of-mass. The real numbers that give the approximate initial position of the probe. Enter (x,y) or (z,r) in units set by *DUnit*. The program locates the element centroid closest to the given point.

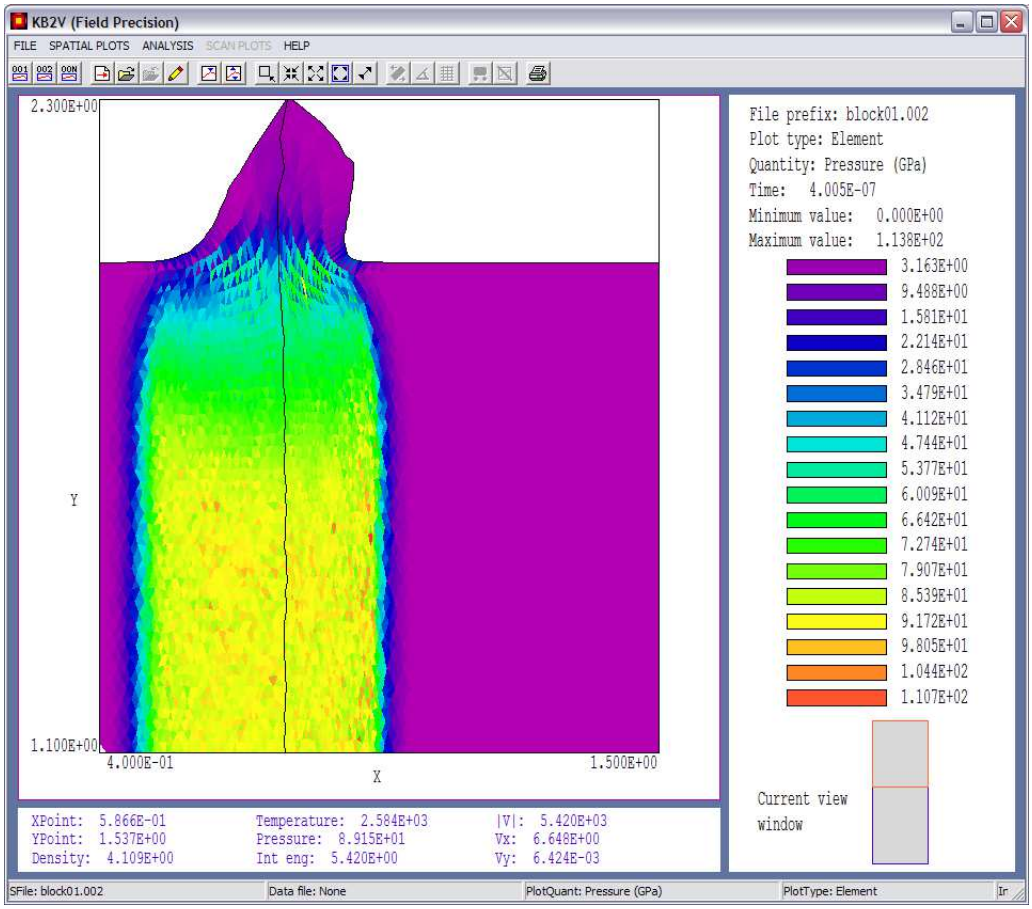

Figure 30: **KB2V** working environment.

9 KB2V

KB2V is an interactive postprocessor to analyze **KB2** solutions. Table 9 lists standard quantities and units. The program menu contains the following main entries: *File*, *Spatial plots*, *Analysis*, *Scan plots*, and *Help*. Initially, only the *File* and *Help* menus are active. You must load data in order to perform analyses and to create plots.

9.1 File menu commands

LOAD FIRST SOLUTION FILE

KB2 generally creates a sequence of data dumps. Use this command to specify a sequence and to load the first file. Changing the directory in the dialog changes the program working directory.

LOAD NEXT SOLUTION FILE

Load the next file in the current sequence. The program displays an error message if you have loaded the last file.

Table 13: **KB2V** standard units

Quantity	**Unit**
Spatial dimensions	meters or units set by *DUnit*
Density, ρ	gm/cm^3
Pressure, p	GPa
Temperature, τ	^{o}K
Internal energy, U	MJ/kg
Velocities	km/s

LOAD SOLUTION FILE NUMBER

Load a specific file in the current sequence. Enter an integer value. For example, the value 13 directs the program to load file `SEQUENCENAME.013`. The program displays an error message if the integer exceeds the highest number in the sequence.

OPEN DATA LISTING FILE

Commands such as *Point calculation* and *Line scan* generate quantitative information. You can automatically record the data generated during an analysis session by opening a data file. Supply a file prefix in the dialog or accept the default. The data file has a name of the form `FPrefix.DAT` and will be stored in the working directory The file is in text format. You can use an editor to view the file or to extract information to send to mathematical analysis programs or spreadsheets.

CLOSE DATA LISTING FILE

Close the current data file. Use this command if you want to start a new file. Note that you must close the data file before opening it with the internal editor.

RUN SCRIPT

A script allows you to perform complex or repetitive analyses on a set of similar solutions. This command displays a dialog listing files with the suffix `SCR`. Pick a file and click *OK*. The script can load data files, open and close data records, and perform any of the quantitative analysis functions described in this chapter. The script command language is described in Sect. 9.5. Note that the analysis script must be in the same directory as the data files.

CREATE SCRIPT

Use this command to create an analysis script with the internal text editor. Supply a file prefix *SPrefix* in the dialog – the resulting script will be saved with the name `SPrefix.SCR`. The program opens the file in the editor and writes a reference list of allowed commands. The list follows the *EndFile* command and will be ignored by the script parser. Enter commands above the *EndFile* command.

EDIT SCRIPT
EDIT DATA FILE
EDIT FILE

Use these commands to view or to modify an existing file. The dialog shows files with suffix `SCR` for the *Edit script* command and `DAT` for the *Edit data file* command. Changing directories in the dialog does not change the working directory of the program.

9.2 Spatial plot menu commands

Spatial plots show variations of of a chosen quantity over the two-dimensional space of the simulation. The following plot types are available:

Mesh. Element facets of the computational mesh.

Regions. Computational mesh with elements color-coded by region number.

Contour. Lines that follow constant values of a computed quantity. In electrostatic solutions, constant values of ϕ are normal to electric field lines. The distance between lines is inversely proportional to the electric field amplitude. Note that contours of $|\mathbf{E}|$ may exhibit regions of compressed lines because the electrical field magnitude is generally not a continuous function in space.

Element. Elements of the solution space color-coded according to a computed quantity (such as the electric field magnitude).

Vector. An element plot with orientation lines included in each element to show the local direction of a vector quantity.

Surface. A three-dimensional plot where a computed quantity is represented as height over a region in the x-y or z-r plane. The spatial limits of the plot correspond to the current view window for *Mesh*, *Region*, *Contour*, *Element* or *Vector* plots. For large meshes, you may notice a delay regenerating a *Surface* plot. The program must map the current quantity to a rectangular grid, performing a large number of interpolations.

The *Settings* popup menu contains the following commands.

PLOT TYPE

Choose the plot type from the above list. A plot type may not support some plotted quantities. For example, a vector plot of pressure is undefined. If you receive a message when you switch plot types that the current quantity is not allowed, use the *Quantity* command to pick a valid option.

PLOTTED QUANTITY

A dialog shows a list of available quantities (Table 9.2) consistent with the current plot type. The command is not active for *Mesh* and *Region* plots

Table 14: **KB2V** plot quantities

Plot type	**Quantity**
Contour	Density, ρ (gm/cm3) Pressure, p (GPa) Temperature, τ (^{o}K) Internal energy, U (MJ/kg) Speed, $\|v\|$ (km/s) Velocity component, v_x or v_z (km/s) Velocity component, v_y or v_r (km/s)
Element	Density, ρ (gm/cm3) Pressure, p (GPa) Temperature, τ (^{o}K) Internal energy, U (MJ/kg) Speed, $\|v\|$ (km/s) Velocity component, v_x or v_z (km/s) Velocity component, v_y or v_r (km/s)
Vector	Velocity component, v_x or v_z (km/s) Velocity component, v_y or v_r (km/s)
Surface	Density, ρ (gm/cm3) Pressure, p (GPa) Temperature, τ (^{o}K) Internal energy, U (MJ/kg) Speed, $\|v\|$ (km/s) Velocity component, v_x or v_z (km/s) Velocity component, v_y or v_r (km/s)
Line scan	Density, ρ (gm/cm3) Pressure, p (GPa) Temperature, τ (^{o}K) Internal energy, U (MJ/kg) Speed, $\|v\|$ (km/s) Velocity component, v_x or v_z (km/s) Velocity component, v_y or v_r (km/s)

PLOT LIMITS

In the default autoscale mode the program picks limits in *Contour*, *Element*, *Vector* and *Surface* plots that span the full range of the current quantity. With this command you can set specific limits. In the dialog uncheck the *Autoscale* box and supply the minimum and maximum values. Note that the program does not check that the values are physically reasonable. This operation will not affect scaling of other plot quantities. Check the box to return to autoscale mode.

TOGGLE GRID

Use this command to activate or to suppress the display of grid lines in *Mesh*, *Region*, *Contour*, *Element* and *Vector* plots. Grid lines corresponding to the axes ($x = 0.0$ or $y = 0.0$) are plotted as solid lines.

SET CONTOUR PLOT STYLE

This command is active only when the current plot type is *Contour*. There are four choices: monochrome, monochrome with labels, colored and colored with labels. In the colored mode, the lines are color-coded according to the value of the plotted quantity. A legend is included in the information window to the right of the plot. In the labeled modes, contour lines are numbered according to their values. Overlapping labels on closely-spaced lines may look better in a zoomed view.

NUMBER OF CONTOURS

Change the number of plotted contour lines. This command is active only when the current plot type is *Contour*.

TOGGLE ELEMENT OUTLINE

This command determines whether the element facets are included in *Element* and *Vector* plots. It may be necessary to deactivate outlines for a clear view of large meshes.

TOGGLE MOUSE/KEYBOARD

By default the program uses interactive mouse entry of coordinates for commands like *Line scan* and *Zoom*. This command switches the program between mouse and keyboard input. Enter keyboard coordinates in the distance units used in **Mesh**. In other words, if the solution program has $DUnit = 1.0 \times 10^6$, then enter dimensions in microns.

TOGGLE SNAP MODE

When snap mode is active, the mouse returns the coordinate values closest to an integer multiple of the quantity *DSnap*. In other words, if $DSnap = 0.5$ and the mouse position is (5.4331, -2.6253), the returned coordinates are (5.500, -2.500). By default, snap mode is active. Snap mode is automatically turned off for coordinate input to the commands *Point calculation* and *Element properties*. Otherwise, the program would pick a location closest to the snap point rather than the tip of the cursor arrow, giving misleading results.

SET DSNAP
Set the distance scale *DSnap* for the mouse snap mode.

TOGGLE FIXED POINT PLOT
In the default mode, **KB2V** creates contour, element and vector plots using element information. Therefore, isolated nodes (representing structures like pressure planes) do not appear. In response to this command, **KB2V** plots circles at fixed-potential nodes that are surrounded by material elements.

The following commands control the size and position of the view in *Mesh*, *Region*, *Contour*, *Element* and *Vector* plots:

ZOOM WINDOW
Zoom in on an area by defining two points of a box with mouse or keyboard entries. When the command is issued, the coordinate mode becomes active.

ZOOM IN
Narrow the view around the current center of the plot.

EXPAND VIEW
Expand the view around the current center of the plot.

GLOBAL VIEW
Expand the view to show the full solution volume rectangle.

PAN
Move the current center of the plot by defining two points of a displacement vector with the mouse or keyboard entries.

The following commands control the appearance of *Surface* plots. The commands are active only when a *Surface* plot is displayed.

FLIP 3D IMAGE
Rotate the *Surface* plot by 90° in the spatial plane.

VIEW ANGLE 3D
Set the elevation angle for the view point.

SET GRID 3D
Change the resolution of the surface plot. To create a *Surface* plot, a quantity is mapped to a

rectangular grid with dimensions $N_x \times N_y$. The numbers also determine the total number of grid lines in the *Surface* plot. The default values are $N_x = N_y = 40$.

The final command group is used to export the current plot to a printer or plot file.

HARDCOPY

This command sends a copy of the current plot to the default Windows printer. If you have several printers, use the *Settings/Printers* option on the Windows Start Menu to make changes in the default before running **KB2V**.

PLOT FILE (EPS)
PLOT FILE (BMP)
PLOT FILE (PNG)

Use this command to create a graphics file of the current plot in either Encapsulated PostScript, Windows Bitmap or Portable Network Graphics formats. The program prompts for a file prefix. The graphics files are created in the current directory with names of the form `FPrefix.EPS`, `FPrefix.BMP` or `FPrefix.PNG`. In some cases, the plot files may not meet your requirements for resolution or clarity. If you have a high resolution display, an effective alternative is to use the screen capture capability of a program like PaintShop Pro. Within the program, you can edit the image, add text, or export to compressed formats like JPEG.

COPY TO CLIPBOARD

Copy the current plot to the Windows clipboard (in Windows Metafile format) where you can paste it into other applications.

9.3 Analysis menu commands

The commands in the *Analysis* popup menu generate numerical data. Most of the functions require coordinate input from the user, usually through the mouse. Therefore, the analysis menu is active only when a *Mesh*, *Region*, *Contour*, *Element* or *Vector* plot is displayed.

POINT CALCULATION

Click on the command and then point to a position in the plot. Note that snap mode is deactivated for coordinate input. The program writes a subset of interpolated quantities to the information area below the plot (Fig 30) and also records complete information if a data file is open. To enter point coordinates by keyboard, use the *Toggle mouse/keyboard* command.

TOGGLE INTERPOLATION

The default interpolation method for the *Point calculation* and *Line scan* commands is a second-order least-squares fit with intelligent collection of data points. For example, only points on the side of a material boundary that contains the target point are included to represent discontinuous quantities correctly at boundaries. The least-squares fit may fail in very small regions or enclosed areas if the program cannot identify enough data points. In this case, toggle

to the linear mode. Here, field values are determined by a first order fit in the element that contains the target point. The status bar reports the current interpolation type.

LINE SCAN

The line scan is one of the most useful functions of **KB2V**. After clicking on the command, supply two points with the mouse in a view of a *Mesh*, *Region*, *Contour*, *Element* or *Vector* plot to define a scan line. The snap mode is useful in this application (for example, you may want a scan to extend from 0.000 to 5.000 rather than 0.067 to 4.985.) The program computes a series of values of field quantities at equal intervals along the line. The information is recorded if a data file is open. The program also makes a screen plot of the currently selected quantity versus distance along the scan and activates the commands in the *Scan plot* menu (Sect. 9.4).

SCAN PLOT QUANTITY

With this command you can choose the quantity to display in screen and hardcopy plots of line scans. Pick the quantity from the list box and click *OK*. This setting has no effect on the data file records which include all field quantities. The available line scan quantities are listed in Table 9.2.

NUMBER OF SCAN POINTS

This command sets the number of line scan points used for the screen plot and recorded in the history file. The default value is 50 and the maximum number is 500.

TOGGLE SYMBOLS

Add or remove plot symbols to show calculated points.

TOGGLE GRID

Add or remove grid lines from the plot.

ELEMENT PROPERTIES

Pick a location with the mouse (or keyboard). **KB2V** highlights the closest element and displays its identity.

REGION PROPERTIES

Pick a location with the mouse (or keyboard) and **KB2V** displays average properties of the surrounding region. The program performs area integrals for rectangular solutions and volume integrals for cylindrical solutions. If a data file is open, **KB2V** makes a listing like the following:

```
 --- Region Information ---
Region No:   2
Material No:   2
Area:   1.746E-04 m2
KEng:   1.108E+06 J/m
IntEng:   1.290E+06 J/m
XAvg:   5.303E-02 m
YAvg:   5.215E-02 m
VxAvg:   1.539E+03 m/s
VyAvg:  -1.804E-02 m/s
Mass:   2.372E-01 kg/m
Exp:  -1.146E+02 m2/s
Number of elements:    20000
RhoAvg:   1.358E+03 kg/m3
PressAvg:   4.134E+09 Pa
XAvg:   5.303E-02 m
YAvg:   5.215E-02 m
```

The quantity *Exp* is the rate of area or volume expansion. A negative number indicates compression.

LINE INTEGRAL

Specify two points with the mouse or keyboard. **KB2V** calculates line integrals of force and mass flux. The force is calculated from the normal component of ∇p. The direction of force is given by

$$F = \int \mathbf{f_n} \times \mathbf{dl}, \tag{52}$$

where $\mathbf{f_n}$ is the normal component of the local force density and **dl** is an element of the line (pointing in the counter-clockwise direction).

VOLUME INTEGRAL

Determine global and regional integrals of the area/volume, kinetic energy and internal energy.

MATRIX FILE

KB2V can make matrix files of hydrodynamic values to help you create your own analysis routines. Although information is available in the output file of the solution program, it may be difficult to deal with the conformal triangular mesh. The *Matrix file* command uses the interpolation capabilities of the program to create a text data file of field quantities on a rectangular grid in x-y or z-r. The command displays a dialog where you set the matrix file prefix, the dimensions of the box and the number of intervals along x and y (or z and r). The program creates the file `FPrefix.MTX` in the current directory. The default is to include all computed quantities.

9.4 Scan plot menu

The commands of the *Scan* menu become active when a plot is created following the *Line scan* command.

OSCILLOSCOPE MODE

In the oscilloscope mode, a scan plot assumes characteristics of a digital oscilloscope. The program superimposes a cross-hair pattern on the graph. Plot values at the intersection are displayed in the information window. Move the marker along the plot by moving the mouse. If you click and hold the left mouse button at a point, the program displays the plot values along with the numerical derivative and integral of the curve. The definite integral is taken from the left-hand side of the plot to the current point. Values are displayed on the screen and written to the data file if open. Press the right mouse button to exit the oscilloscope mode.

CLOSE SCAN PLOT

The scan plot must be closed before you can use the *File* and *Analysis* functions of **KB2V**. This command closes the scan plot and returns the program to the previous spatial plot.

9.5 Analysis script commands

Scripts to control analysis sessions have a name of the form `FPrefix.SCR`. They should be in the same directory as the data files. Scripts are text files that follow the syntax conventions of the solution program input scripts (Sect. 6.4). Data lines use the standard delimiters and comment lines begin with an asterisk [*]. Processing ends when the *EndFile* command is encountered.

To run a script, choose the *Run script* command in the *File* menu. The program shows a list of available scripts. Pick a file and click *OK*. The script operates on the presently loaded data file or you can load other files from within the script. You can also sequentially open one or more data files.

KB2V can perform analyses autonomously under script file control from the command prompt. If the file `GTest.SCR` is in the data directory, then use a command of the form

```
[ProgPath]\KB2V GTEST <Enter>
```

The main application of the command prompt mode is to generate data files and to perform extended analyses under batch file control.

The following commands may appear in a script:

INPUT FileName
INPUT Switch1.001

Close the current data file and load a file for analysis. The parameter is the full name of the data file. For the command illustrated, the post-processor would load the file `SWitch1.001`. You can load several files for sequential analysis.

OUTPUT FPrefix
OUTPUT SW02

Close the current data file and open an output file `SW02.DAT`.

NSCAN NScan
NSCAN = 150
Set the number of points in a line scan. The default is 50 and the maximum number is 500.

INTEPOLATION [FIRST,SECOND]
INTERPOLATION = Linear
Set the method for interpolation of the KB tables.

POINT X Y
POINT Z R
POINT = (5.65, 10.68)
Perform interpolations at the specified point and write the results to the data file. The two real number parameters are the coordinates of the point in **Mesh** units.

SCAN Xs Ys Xe Ye
SCAN Zs Rs Ze Re
SCAN = (0.00, 0.00) (10.00, 0.00)
Write the results of a line scan between the specified points to the data file. The four real number parameters are the starting and end coordinates in **Mesh** units.

ELEMENT X Y
ELEMENT Z R
ELEMENT = (5.65, 10.68)
Write the properties of the element at the specified point to the data file. The two real number parameters are the coordinates of the point in **Mesh** units.

REGION RegNo
REGION = 5
Write volume and surface integrals for a region to the data file. The integer parameter is the region number.

LINEINT Xs Ys Xe Ye
LINEINT Zs Rs Ze Re
LINEINT = (0.00, 0.00) (10.00, 0.00)
Write line integrals along a scan line to the data file. The four real number parameters are the starting and end coordinates in **Mesh** units.

VOLUMEINT
Write volume integrals for the full solution and regions to the data file.

MATRIX FPrefix Nx Ny Xs Ys Xe Ye
MATRIX FPrefix Nz Nr Zs Rs Ze Re
MATRIX = Switch1 (10, 20) (0.00, 0.00, 5.00, 10.00)

Open a matrix file and record values. The command requires seven parameters: 1) The prefix of the matrix file `FPrefix.MTX` (string), 2) the number of intervals along the x or z direction (integer). 3) the number of intervals along the y or r direction (integer), 4-7) coordinates of the corners of a box in the solution volume (real).

The following is an example of a script to compare hydrodynamic values along the axes of four different solutions and to write the results to the file `COMP.DAT`.

```
NSCAN 200
OUTPUT COMP
INPUT SWITCH01.001
SCAN 0.00 -50.00 0.00 50.00
INPUT SWITCH02.001
SCAN 0.00 -50.00 0.00 50.00
INPUT SWITCH03.001
SCAN 0.00 -50.00 0.00 50.00
INPUT SWITCH04.001
SCAN 0.00 -50.00 0.00 50.00
ENDFILE
```

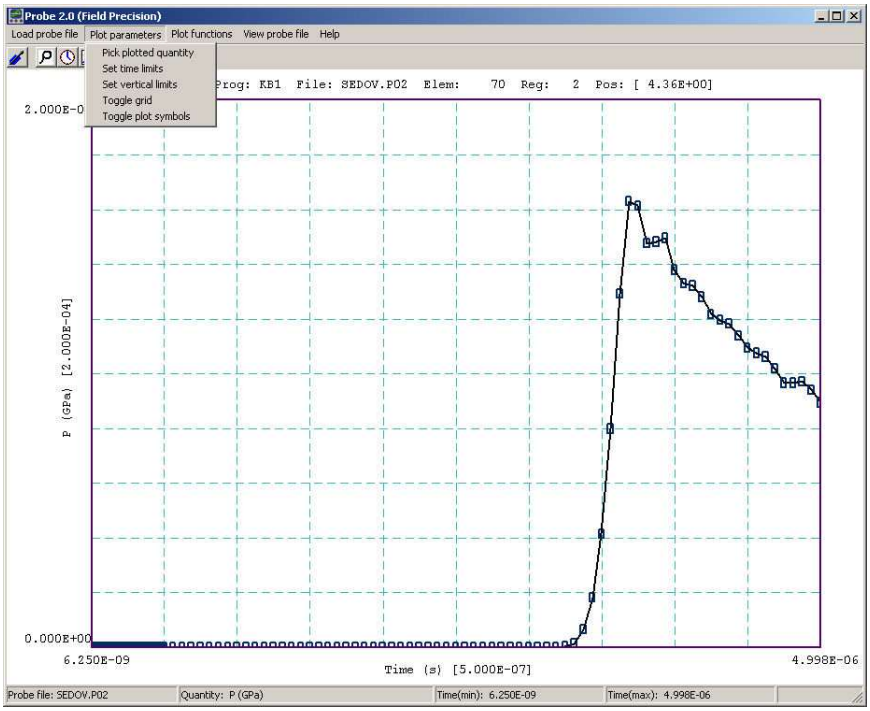

Figure 31: **Probe** screen shot.

10 Probe – history file plot utility

10.1 Introduction

Probe is the universal plotting program for all Field Precision initial-value solution codes. You can set from 1 to 20 probes by specifying positions in the solution program command script. The probes record quantities in an element or at a node as a function of time. The resulting text files have names of the form `FPREFIX.P01`,..., `FPREFIX.P12`, where `FPREFIX` is the run prefix.

Table 15 shows the standard probe file format. The first section is a header that contains the following information:

Generating program name.

Dimensionality of the generating program (1, 2 or 3).

The spatial position of the probe (from 1 to 3 quantities).

The index of the element sampled by the probe.

The region number of the element.

Conversion factors for the probe position and the recorded quantities.

Labels for the recorded quantities.

Although the solution programs and their output files employ SI units (meters, kilograms,...), the graphical analysis displays often use practical units to make it easier to visualize results and to facilitate automatic grids. **Probe** multiplies file quantities by the conversion factors during the loading process. Note that the quantity *DConv* and conversion factors for positions are equal to *DUnit*, a variable used in many solution programs. After four lines of label information, the remainder of the file consists of data lines. Each line contains the time (in seconds) and one or more element or node quantities. Real numbers are recorded in E15.6 format.

10.2 Loading data files

When you start **Probe** the only active menu option is *Load probe*. Plotting and analysis functions become active when a probe file has been opened. The program displays a dialog showing all files with suffixes of the form `P01`,...,`P12`. Pick a file to analyze and click *OK*. Changing directories in the dialog will change the working directory of the program. If the load is successful, **Probe** creates a default plot of the data (Fig. 31).

The status bar at the bottom of the window contains the name of the probe file, the current plot quantity, and the temporal range of data. The default plot shows the first quantity recorded in the probe file over the full range of time. The horizontal and vertical scales are chosen so that the plot fits on the screen and the grid lines are automatically adjusted so that they lie on even values of the plotted quantity with easily recognized intervals (*e.g.*, 0.02, 0.05, 0.10, ...). The grid intervals are shown in parentheses next to the labels of the horizontal and vertical axes. The title line at the top of the plot shows the following information: generating program, probe file name, element number, region number and position. This information is recorded in hardcopy plots to help you archive your data.

10.3 Plot settings

The commands of the *Plotsettings* menu control the quantities, ranges and appearance of the plot. The screen plot automatically updates whenever you make a change.

PLOTTED QUANTITY

A dialog shows a list of element quantities included in the probe file. Highlight your choice and click *OK*.

TIME LIMITS

By default **Probe** shows the full time-span recorded. You can narrow the range by supplying values for the minimum and maximum time. Uncheck *Autoscale* in the dialog and supply maximum and minimum values. To return to the full range, check the *Autoscale* box.

VERTICAL LIMITS

In the default mode **Probe** picks a scale to display the full range of the plotted quantity. You can narrow or expand the range by supplying minimum and maximum values. The program returns to full range if you check the *Autoscale* box or if you change quantities using *Pick plotted quantity*.

Table 15: Example of the **Probe** file format

```
Field Precision probe file
Program: KB1
NDimen: 1
XPosition:   4.357E-02
ElementNo:    70
RegionNo:   2
NQuant: 6
DConv: 100.0
QConv1: 100.0
QConv2: 0.001
QConv3: 1.0E-9
QConv4: 1.0
QConv5: 1.0E-6
QConv6: 0.001
QLabel1: x or r (cm)
QLabel2: Rho (gm/cm3)
QLabel3: P (GPa)
QLabel4: T (deg-K)
QLabel5: U (MJ/kg)
QLabel6: v (km/s)

       Time             Re              Rho            Press
        (s)             (m)          (kg/m3)          (Pa)
  ============================================================
   6.250000E-09   4.357041E-02   1.000000E-01  -1.238464E+02
   1.250000E-08   4.357041E-02   1.000000E-01  -1.238464E+02
   1.874999E-08   4.357041E-02   1.000000E-01  -1.238464E+02
   2.499996E-08   4.357041E-02   1.000000E-01  -1.238464E+02
   3.124995E-08   4.357041E-02   1.000000E-01  -1.238464E+02
   ...

            Temp           Epsi            V(Av)
          (deg-K)         (J/kg)          (m/s)
    ============================================
       1.000000E-03   8.620001E+00   0.000000E+00
       1.000000E-03   8.620001E+00   0.000000E+00
       1.000000E-03   8.620001E+00   0.000000E+00
       1.000000E-03   8.620001E+00   0.000000E+00
       1.000000E-03   8.620001E+00   0.000000E+00
       ...
```

TOGGLE GRID
Switch between grid and and fiducial lines in the plot.

TOGGLE PLOT SYMBOLS
Include or remove symbols to mark the recorded points.

10.4 Plot functions

The commands of the *Plot functions* menu activate the *Oscilloscope mode* of the program and also send plots to hardcopy devices or plot files.

OSCILLOSCOPE MODE
When you issue this command, **Probe** simulates a digital oscilloscope. As shown in Fig. 32, the mouse cursor changes to a cross-hair pattern when it is inside the plot window. The program adds movable fiducial lines to mark the current point. You can drag the fiducials along the time axis by moving the mouse. A box at the bottom of the plot shows values of the time and plotted quantity at the current position. If you press the left mouse button, the program displays a box with the following information about the current point:

Time, t.

Value of the plotted quantity, $V(t)$.

Derivative of the plotted quantity, $dV(t)/dt$.

Definite integral of the plotted quantity, $\int_0^t V(t')dt'$.

The definite integral is taken from the time of the first recorded value in the probe file to that of the current point. You can find integrals between points by subtracting values. Other functions of the program are deactivated in the *Oscilloscope mode*. Press the right mouse button or the *Esc* key to return to normal program operation.

SMOOTH DISPLAY
Use this command one or more times to smooth the currently-displayed trace. Smoothing applies to the screen display and exported plots, but does not affect the data values in the probe file.

DEFAULT PRINTER
Probe can port copies of the plot to any installed Windows printer. The program sends output to the default printer, so be sure to select the correct device using the *Settings/Printer* function of Windows before making the plot.

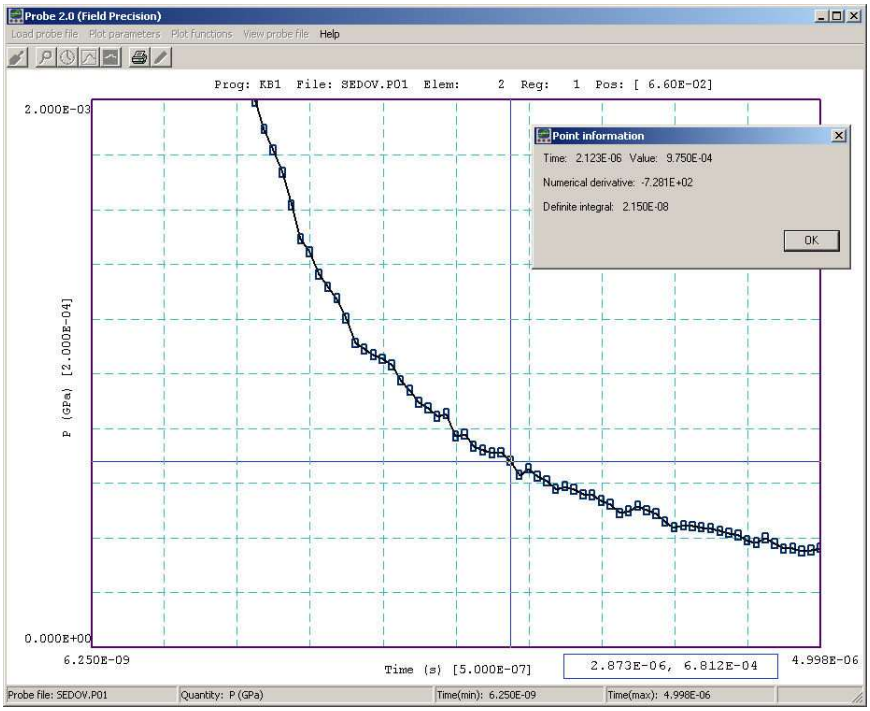

Figure 32: **Probe** in the *Oscilloscope mode*.

PLOT FILE (EPS)
PLOT FILE (BMP)
PLOT FILE (PNG)

Send the plot to a file in the following formats: Encapsulated PostScript, Windows Bitmap or Portable Network Graphics. The program prompts for a file prefix and then creates a file with the names `FPREFIX.EPS`, `FPREFIX.BMP` or `FPREFIX.PNG`.

COPY TO CLIPBOARD

Copy the plot to the clipboard in in Windows MetaFile format.

10.5 Information

PROBE FILE INFORMATION

Display information on the probe file in a message box (Fig 33). The quantity $NSkip$ in line 7 is used for long files. There is no reason to store more than 1000 points for plots on typical screens and hardcopy devices. When there are less than 1000 data lines, **Probe** loads all points ($NSkip = 1$). When the file contains 1000 to 2000 data lines, the program loads every second point ($NSkip = 2$), and so forth. In this way the **Probe** can handle probe files of any length without exceeding memory limits.

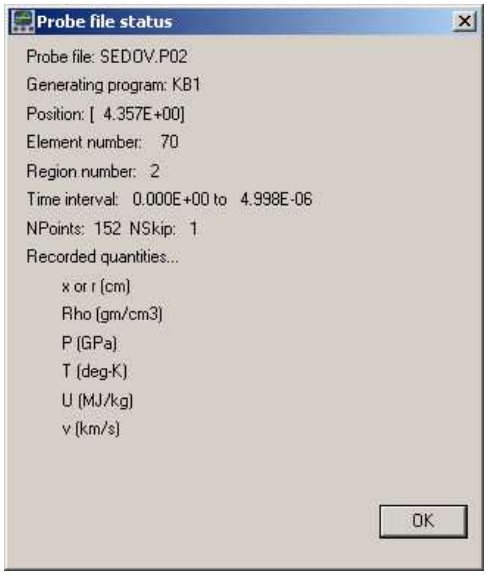

Figure 33: **Probe** file-information message box.

VIEW PROBE FILES

Load a probe file into the internal editor so you can inspect the data directly. The editor runs in read-only mode so that you cannot change the file. Exit the editor to return to program operation.

PROBE MANUAL

Show this document in your default PDF viewer.

11 KBLaunch – advanced features

The KB program launcher (`kb.exe`) helps you to organize your work in two ways:

- Only one shortcut is required on your desktop, minimizing clutter.
- All programs open in a specified data directory, eliminating redundant trips through the directory tree.

Another function is the organization of extended calculations in the background.

11.1 Setting the program and data directories

Figure 1 shows the screen display of the **KBLaunch** controller. To begin, click the *Program folder* button in the *Control* group. In the dialog move to the directory that contains the executables and click *OK*. The default location is `c:\fieldp\kb`. The buttons in the technical group should all become active. An inactive button indicates a missing executable.

It is a good practice is to collect all input and output files for related **KB** solutions in a specific data directory. Use the *Data Folder* button to set the current location. Programs that are opened after the change will read and write to the directory. (Note that the setting does not affect previously-opened programs.) The *Information* area at the bottom of the control box shows: 1) the current data directory, 2) the last operation performed and 3) the program directory.

11.2 Creating and running tasks

KB programs are optimized for the latest generation of multi-core or multi-processor PCs. A useful feature programs is the capability to run multiple calculations simultaneously. All solution programs can run in the background if launched from a Windows batch file. Background operation is automatic and faster than running in a window. The *Create task* and *Run task* commands in **KBLaunch** make it easy to use batch files. With the commands you can 1) quickly define multi-step calculations (*tasks*) in an interactive dialog, 2) launch simultaneous tasks in the background and 3) find out which tasks are running.

The *Create task* button calls up the dialog of Figure 34. Supply a file prefix `FPREFIX` that indicates the function of the task. The task information will be stored in a DOS batch file `FPREFIX.BAT` created in the current **KB** data directory. Commands in the file are compatible with all recent Windows versions including Windows 7. Each row represents an operation (batch file command). The first column defines the action. Clicking on a cell brings up a menu that includes all **KB** programs capable of background operation. In addition, several relatively safe DOS commands are included (`ERASE`, `COPY`, `MOVE`, `RENAME` and `REM`). All commands operate on a file (*FileIn* column). The DOS commands `COPY`, `MOVE` and `RENAME` require a second file name (*FileOut* column). You can type file names in the cells. By default, the files are in the **KB** working directory, but you can include path information if the files are in other directories. Alternatively, you can click in a cell and then pick the *Select file* command to use the standard Windows dialog for choosing files anywhere on the computer. For the **KB** programs, the dialog displays only files with appropriate suffixes (*e.g.*, `*.KIN` for **KB1**).

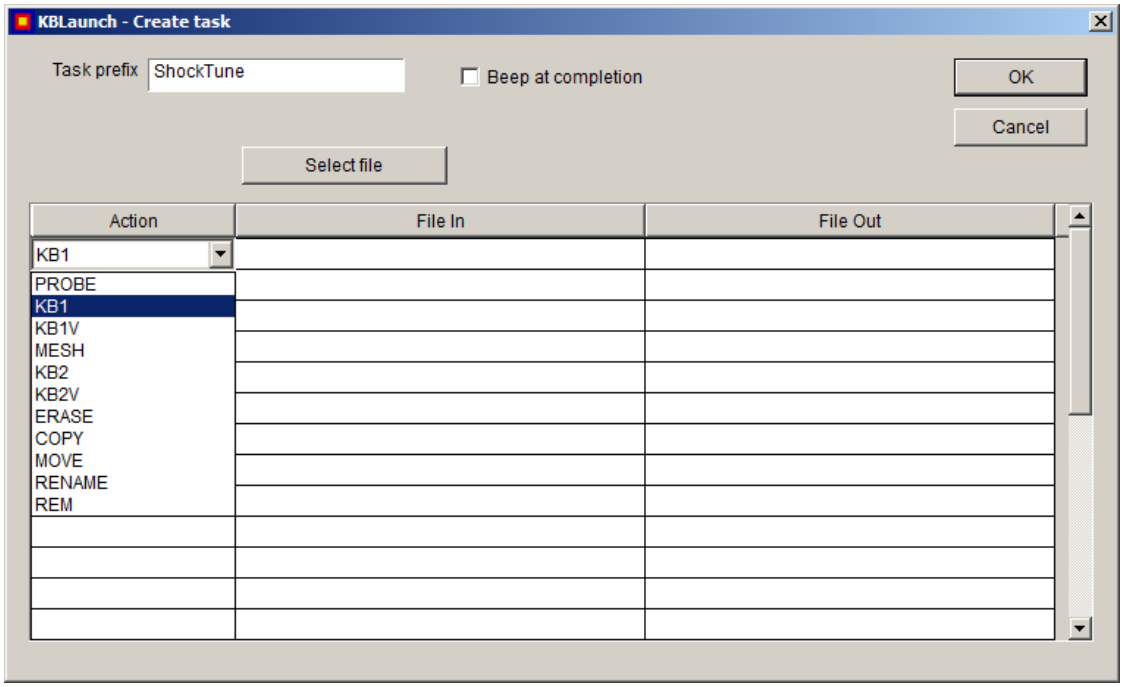

Figure 34: Create task dialog

Click the *OK* button when the sequence is complete to create the batch file. Here is an example:

```
REM KB batch file, Field Precision
START /B /WAIT C:\fieldp\kb\mesh.exe C:\Temp\convergegun
START /B /WAIT C:\fieldp\kb\kb2.exe C:\Temp\convergegun
START /B /WAIT C:\fieldp\kb\kb2v.exe C:\Temp\convergegun
ERASE *.?ls
START /B /WAIT C:\fieldp\kb\notify.exe
IF EXIST Electrode01.ACTIVE ERASE Electrode01.ACTIVE
```

The operations listed perform a complete **KB** calculation in the background and then erase all listing files. The example has some notable features:

- The operations are performed sequentially because data from one operation may be used in the next. To run calculations in parallel, define and run multiple tasks.
- You can modify the file with an editor if you are familiar with DOS commands.
- The DOS commands recognize the standard wildcard conventions (* for any character grouping, ? for any character).
- The programs adds the command `notify.exe` to the task sequence if *Audio alarm* was checked. In this case, the computer beeps when a task is completed.
- The final command to erase a file `FPREFIX.ACTIVE` is added to all batch files. The presence of the file indicates that the task is running.

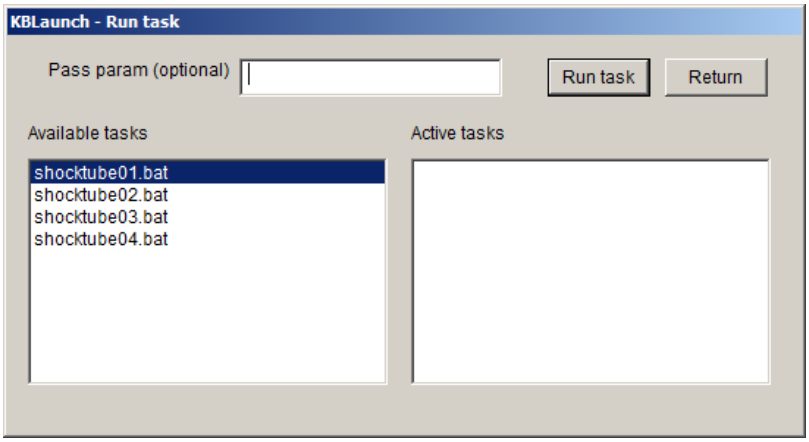

Figure 35: Run task dialog

Click the *Run task* button when you have created tasks or moved predefined task files to the data directory. The dialog (Figure 35) organizes tasks into two groups: ones that are available to run and ones that are currently running (*i.e.*, `FPREFIX.ACTIVE` has been detected). To launch a task, choose one from the top list and click *OK*. The program creates a file `FPREFIX.ACTIVE` and runs the batch file. The program sequence runs silently in the background. In the meantime, you can prepare other inputs or run other tasks.

11.3 Tools

You will probably use additional software tools working with **KB** and other technical programs. You can set **KB** to launch your favorite utility programs. To define a text editor, press the *Setup tools* button in the *Control* section. In the dialog, choose the *Editor* option. Then, move to the appropriate directory and select the program. When you exit the procedure, the *Editor* button in the *Tools* section becomes active.
You can use the *Set tools* command to define two other utilities. For the *File manager* option, select a program like **Windows Explorer** or **FreeCommander**. Use the *Data analysis* button for a spreadsheet, plotting program or mathematical analysis software. The textitCommand button opens a DOS window if you want to run programs from the command prompt or under the control of your own batch files.

12 KB tutorials

12.1 One-dimensional shock resulting from the collision of slabs

This **KB1** calculation models a planar shock resulting from the impact of a moving slab striking a stationary target. An aluminum slab of thickness 0.5 cm moving at $v_0 = 10$ km/s strikes a Lucite target of thickness 1.0 cm. We can predict the properties of shocks moving into the materials from the contact point using the shock conservation equations (Sect, 2.2). A shock wave propagates into the Lucite with pressure p_2 and particle velocity u_{p2}. Similarly, a shock propagates backward in the aluminum with pressure p_1 and particle velocity -u_{p1} relative to the moving medium. Two conditions must be satisfied at the contact point between the materials:

The pressures are equal, $p_1 = p_2$.

The particle velocities in the stationary frame are equal, $u_{p2} = v_0 - u_{p1}$.

These conditions, combined with the Hugoniot relationships, define unique shock states in both materials.

One way to find the state is to plot the Hugoniot curve $p(u_{p1})$ and the shifted curve $p_2(v_0 - u_{p2})$ and identify the intersection. Using **KBTView** to generate Hugoniot curves for the materials `ALUM3715` and `LUCT7750` leads to the plot of Fig. 36. The common point corresponds to the following shock parameters: $p_1 = p_2 = 91$ GPa, $u_{p2} = 6.62$ km/s and $u_{p1} = 3.38$ km/s. The predicted shock velocity in Lucite with a density of $\rho_2 = 1186$ kg/m^3 is $u_s = p_2/\rho_2 u_{p2} = 11.6$ km/s. The shock velocity in the rest frame of the aluminum ($\rho_1 = 2700$ kg/m3) is $u_s = p_1/\rho_1 u + p1 = 9.97$ km/s. Therefore, the shock front velocity in the stationary frame is 0.03 km/s.

The files `SLAB01.KIN`, `ALUM3715.KBT` and `LUCT7750.KBT` are required for the calculation. The **KB1** control file `SLAB01.KIN` is listed in Table 16. The contact point is initially at position $x = 0.5$ cm. Figure 37 shows the calculated pressure profile 350 ns after contact. Filled squares indicate the positions of aluminum elements and filled circles represent Lucite. The predicted positions of the shock fronts are 0.906 cm in the Lucite and 0.501 cm in the aluminum. The code values for pressure and shock positions agree well with the predictions.

Table 16: File SLAB01.KIN

```
* File SLAB01.KIN
* ------------------ Run control --------------------
  GEOMETRY: RECT
  DT: 0.25E-9
  TMAX: 500.0E-9
* -------------- Material properties ----------------
  MATERIAL 1 KBT ALUM3715
  MATERIAL 2 KBT LUCT7750
* -------------------- Geometry ----------------------
* Aluminum flyer plate
  REGION 1 1 0.000 0.005  40
* Lucite target
  REGION 2 2 0.005 0.015  80
* --------------- Region properties -----------------
  VISCOSITY 1 5.0
  VELINIT 1  1.0E4
  HYDINIT 1 2.7000E+03 298.0
  VISCOSITY 2 5.0
  VELINIT 2 0.0
  HYDINIT 2 1.1860E+03 298.0
* ------------------ Diagnostics --------------------
  DTIME 50.0E-9
ENDFILE
```

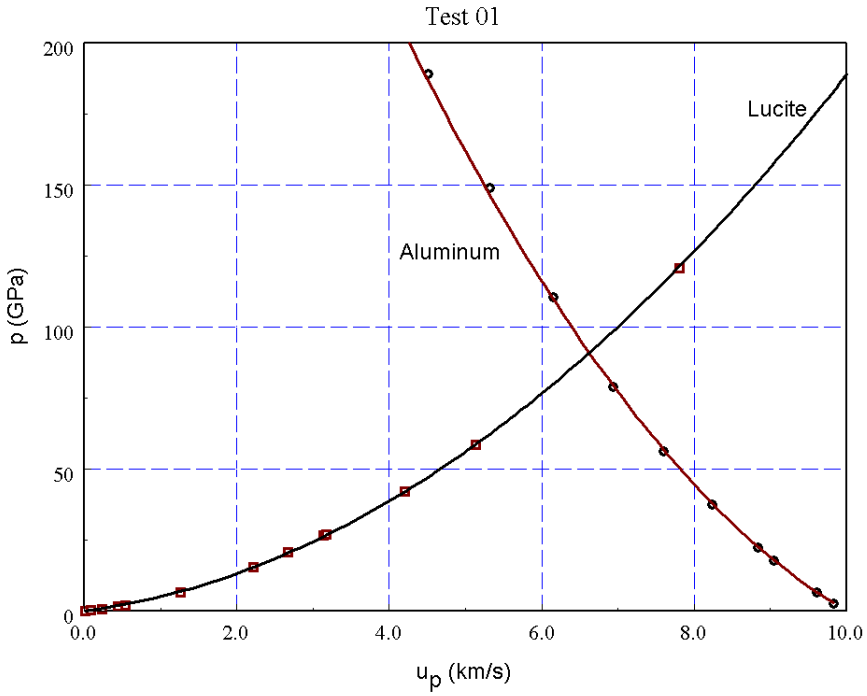

Figure 36: Tutorial 1: calculation of shock parameters from the Hugoniot curves.

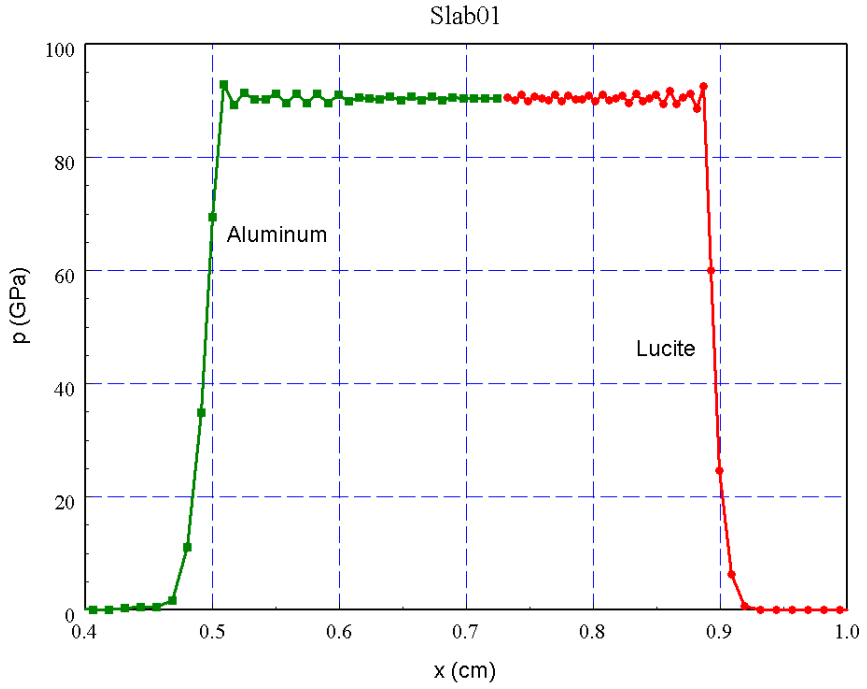

Figure 37: Tutorial 1: pressure profile at 350 ns.

12.2 Planar detonation wave in Composition B

In this **KB1** simulation the impact of a thin aluminum on a slab of the explosive Composition B initiates a planar detonation wave. We can compare results with the predictions of Section 2.3. The input files are `PLANEDET.KIN` and `ALUM3715.KBT`. The input script file has the contents:

```
GEOMETRY: RECT
DT: 1.0E-9
TMAX: 10.1E-6
MATERIAL 1 KBT ALUM3715
MATERIAL 2 EXPL 1.56E3 2.46E3 3.52 -8.810E-4 2.0E10 5.183E6 2.63
REGION 1 1 -0.001 0.000    2
REGION 2 2  0.000 0.100  200
VISCOSITY 1 5.0
VISCOSITY 2 5.0
VELINIT 1 8.0E3
DTIME 2.00E-6
SETPROBE 3
PROBESTEP 1
```

Line 5 defines properties of Composition B. The explosive has $\rho = 1561$ kg/m^3, Q = 5.186 M/kg and $\gamma = 2.63$. The predicted Chapman-Jouguet pressure (Eq. 36)is $p_{CJ} = 26.4$ GPa. The initiation pressure is set at 20 GPa, a value somewhat less than p_{CJ}. The equations of Sect. 2.3 give the following values for other material parameters at the CJ point: $u_d = 7.83$ km/s, $u_p = 2.16$ km/s, $U = 7.51$ MJ/kg and $\rho = 2154$ kg/m^3.

The explosive has a thickness of 10 cm. During the 10 μs run the detonation front should move 7.83 cm. A probe is placed in the first element to check conditions for detonation. The aluminum plate (Region 1) is 1 mm thick. No detonation wave is observed for plate velocities less than 4 km/s. At the critical velocity of 4 km/s, the first element of the Composition B reaches 20 GPa at 85 ns after contact. At this time, the particle velocity u_p in the element is 1.9 km/s, close to the CJ value. A incident velocity of 8 km/s was used in the production run for fast initiation. In this case, the first element detonated 15 ns after impact.

The spatial variation of pressure in Figure 38 (10 μs after initiation) follows the expected behavior of an ideal detonation wave[6]. The code gives the following parameters at the CJ point, in agreement with predictions:

Pressure: 26.4 GPa
Position at 10 μs: 7.78 cm
Inferred detonation velocity, u_d: 7.78 km/s
Density, ρ: 2158 kg/m3
Internal energy, U: 7.51 MJ/kg
Particle velocity, u_p: 2.17 km/s

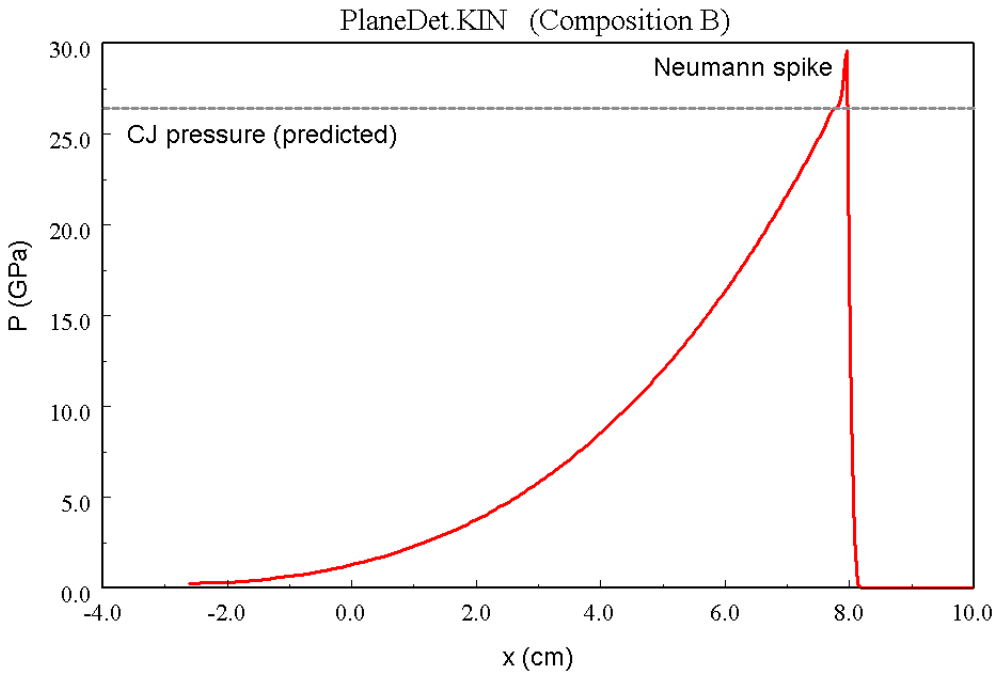

Figure 38: Tutorial 2: spatial variation of pressure at 10 μs.

12.3 Compression shock in an ideal gas

We use **KB1** to model a standard hydrodynamic test, initiation of a shock by a uniform-velocity compression of an ideal gas. The simulation illustrates comparisons between the ideal gas and the **KB** table material models as well as the relative accuracy of **KB** interpolations. In the model an ideal gas with $\gamma = 5/3$ has an initial uniform density ρ_0. At all positions the gas has an initial velocity v_0 directed toward a cylindrical axis. For the cylindrical geometry, hydrodynamic theory predicts that a shock wave with density $16\rho_0$ propagates outward from the axis with a velocity $u_s = v_0/3$. Table tab:tut03 shows the input script `NOHCYL02.KIN`. Note that alternative run parameters are shown as comments.

Figure 39 shows results. The red line is a superposition of results using a *Gamma* material with $\gamma = 5.3$ or the **KB** table `IGAS0001.KBT` with initial density 1.0 kg/m^3. The two models give almost identical results and are in good agreement with theory. The predicted position of the shock front at 6.0 μs is 0.200 cm. The discrepancy from the ideal model near the axis is a feature that appears in all numerical hydrodynamic models Because the initial pressure is zero, there is no mathematical path to convert the gas kinetic energy to internal energy in the absence of artificial viscosity. The introduction of artificial viscosity resolves the problem, but causes a dip in density and elevated temperature at the turning point. The pressure has the approximately uniform value 5.3×10^6 Pa behind the shock. Note that the density in front of the shock is higher than the initial value. A uniform velocity (independent of r directed toward the axis puts the material into compression, even in the absence of the shock.

You can try alternate geometries. For the planar case, the node at $x = 0.0$ is anchored (symmetry boundary). Theory predicts that u_s should be the same for planar, cylindrical and spherical systems. Density values behind the shock are predicted to have the following values:

Table 17: File NOHCYL02.KIN

```
* --- RUN CONTROLS ---
* (Test the geometry)
  GEOMETRY: CYLIN
*  GEOMETRY: PLANE
*  FIXBOUND: IN
*  GEOMETRY: SPHERE
  DT: 1.0E-9
  DTCHANGE: 0.5E-6 2.50E-9
  TMAX:  6.01E-6
* (Test the interpolation accuracy)
*  INTERPORDER FIRST
*  INTERPORDER SECOND
* --- MATERIAL PROPERTIES ---
* (Test the material model)
  MATERIAL 1 GAMMA  1.000  1.6667
*  MATERIAL 1 KBT  IGAS0002
* --- GEOMETRY ---
  REGION  1  1  0.0000 0.0100  250
* --- REGION PROPERTIES ---
  HYDINIT 1  1.000  0.001
  VELINIT 1 -1000.0
  VISCOSITY 1  2.00
* --- DIAGNOSTICS ---
  PROBESTEP 10
  SETPROBE 56
  DIAGTIME 3.00E-6
  DIAGTIME 6.00E-6
ENDFILE
```

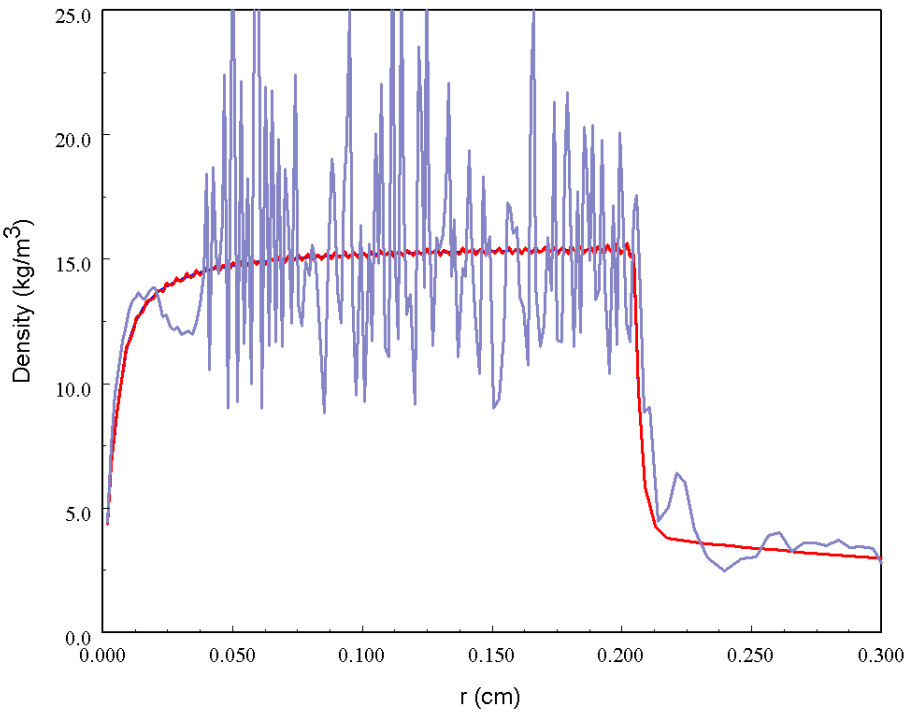

Figure 39: Tutorial 3: spatial variation of density at 6.0 μs. Red: Results for a γ law material model and for second-order interpolation on the **KB** table `IGAS0001.KBT`. Blue: first order interpolation on the **KB** table.

$4\rho_0$ for planar, $16\rho_0$ for cylindrical and $64\rho_0$ for spherical geometry.

The time for the run with the **KB** table is about 20 times that with the analytical model. The difference reflects the extra work involved in the second-order interpolations. This run severely tests the interpolation routines. The final element temperature of 60 °K is smaller than the first tabulated temperature of 100 °K in `IGAS0001`. For this reason, the first-order interpolation performs poorly (blue line in Fig. 39). This is an unusual case. It is important to note that first order interpolation usually give sufficient accuracy in more common runs with high shock temperatures.

12.4 Sedov blast wave

The Sedov blast wave is an analytic solution for the propagation of a spherical shock in a uniform ideal gas. The shock is initiated by a delta-function distribution of internal energy at the origin. The theory is described in Ya. B. Zel'dovich and Yu. P. Raizer, **Physics of Shock Waves and High-temperature Hydrodynamic Phenomena** (Academic Press, New York, 1966), 93.

Consider a uniform ideal gas described by the parameter γ with initial density ρ_0. A total energy E_0 is deposited near the origin. The radius of the spherical shock as a function of time is given by

$$r = \zeta_0 \left(\frac{E_0}{\rho_0} \right)^{1/5} t^{2/5}. \tag{53}$$

For the choice $\gamma = 5/3$, the factor in the equation is $\zeta_0 = 1.15$. The shock velocity is

$$u_s = \frac{2}{5} \zeta_0^{5/2} \left(\frac{E_0}{\rho_0} \right)^{1/2} r^{-3/2}. \tag{54}$$

The predicted density and pressure immediately behind the shock front are given by

$$\rho_s = \rho_0 \left(\frac{\gamma + 1}{\gamma - 1} \right), \tag{55}$$

$$p_s = \rho_0 u_s^2 \left(\frac{2}{\gamma + 1} \right). \tag{56}$$

In the **KB1** calculation `SEDOV.KIN`, we can use either the *Gamma* model or the **KB** table `IGAS002.KBT`. Table 18 shows the input file. The zero temperature gas with density $\rho 0 = 0.1$ kg/m^3 extends to a radius of 6 cm. The point source of energy is represented by a region of radius 2 mm with a uniform internal energy. The choice of total energy $E_0 = 617$ J gives a shock radius of $r = 5.0$ cm at $t = 5.0 \mu$s. The mass of the central region is 3.351×10^{-9} kg, giving an initial internal energy of $U_0 = 1.84 \times 10^{11}$ J/kg. The theoretical values of density and pressure at the shock front are $\rho_s = 0.4$ kg/m^3 and $p_s = 1.19 \times 10^6$ Pa. Figure 40 shows the spatial variation of density and pressure at 5 μs. The shock position and values of ρ_s and p_s are in agreement with theory.

Table 18: Contents of file SEDOV.KIN

```
TITLE Sedov blast wave
*
* --- RUN CONTROL ---
GEOMETRY: SPHERE
*  INTERPORDER: SECOND
DT: 0.25E-9
DTCHANGE 0.5E-6 2.5E-9
TMAX:  5.01E-6
* --- MATERIAL PROPERTIES ---
*  MATERIAL 1 KBT IGAS0002
MATERIAL 1 GAMMA 1.66667
* --- GEOMETRY ---
REGION  1  1  0.0000 0.002 5
REGION  2  1  0.0020 0.060 90
* --- REGION PROPERTIES ---
*  HYDINIT 1  0.1000 2.135E7
HYDINIT 1  0.1000 1.84E11
VISCOSITY 1 2.50
*  HYDINIT 2  0.1000 0.001
HYDINIT 2  0.1000 0.000
VISCOSITY 2 2.50
* --- CONTROL ---
  DIAGTIME: 5.0E-6
  PROBESTEP: 25
  SETPROBE: 70
ENDFILE
```

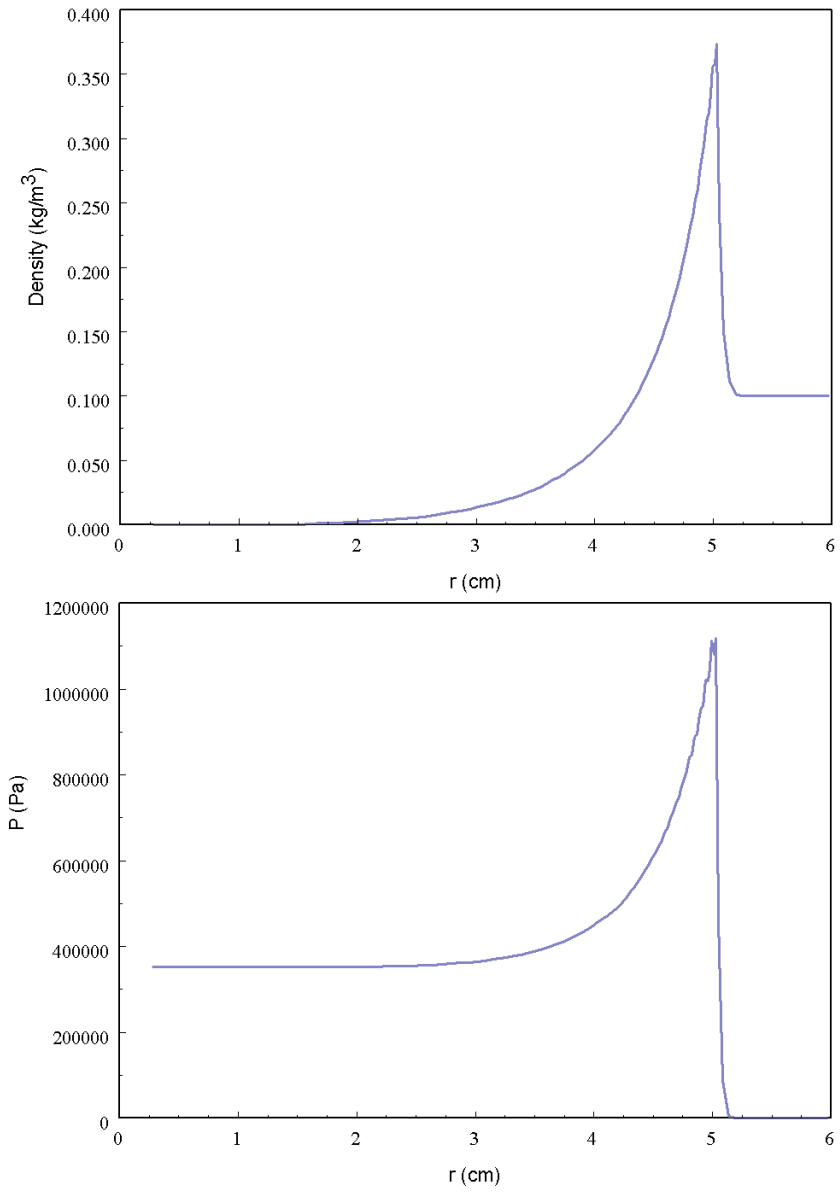

Figure 40: Tutorial 4: Sedov blast wave, conditions at 5.0 μs. Top: density. Botton: pressure.

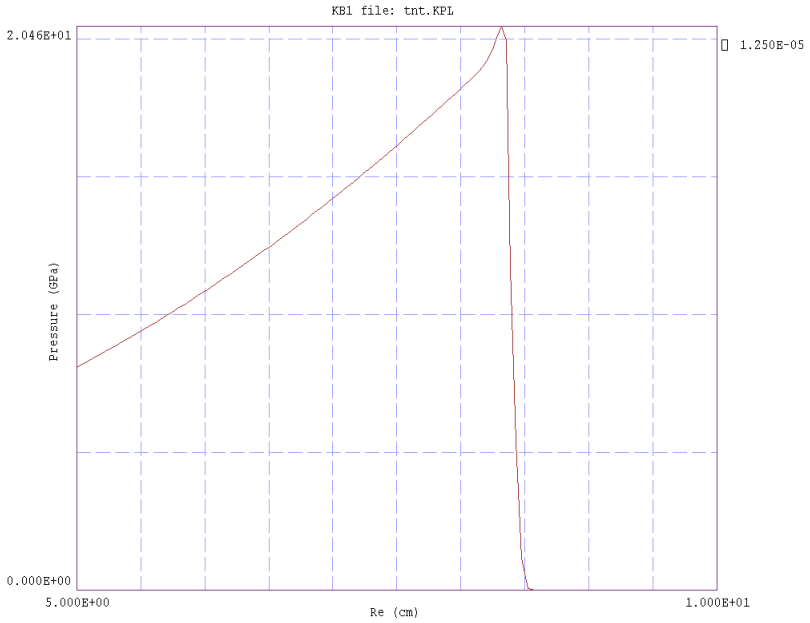

Figure 41: Pressure profile of a planar detonation wave in TNT 12.5 μs after ignition. Predicted front position: 8.38 cm.Predicted CJ pressure: 19.5G Pa. Note the Neumann pressure spike at the front.

12.5 Detonation of a TNT rod

This tutorial demonstrates the accuracy of KB2 for modeling explosive materials.The simulations address the detonation of unconfined rods of TNT.The KB detonation model was discussed in Sect. 2.3. The following parameters for TNT are listed in the appendix: $\rho_0 = 1.50 \times 10^3$ kg/m, $Q = 4.51 \times 10^6$ J/kg, $\gamma = 2.44$, $C_0 = 1.975 \times 10^3$ m/s, $S_1 = 3.014$ and $S_2 = -6.024 \times 10^{-4}$ s/m. The quantity p_{init} is the only adjustable parameter in the detonation model. It specifies the pressure at which an element detonates. For homogeneous explosives, p_{init} should be close to p_{CL}, the Chapman-Jouguet pressure. For inhomogeneous explosives with possible hot spots, lower values may be appropriate. The value $p_{init} = 0.75 p_{CL}$ was used in these calculations.

Equations 34, 35 and eq:pcj give the material state at the Chapman-Jouguet point of a planar detonation wave in an infinite medium. The CJ point refers to the equilibrium state of exploded material at the detonation front just behind the thin Neumann pressure spike.The following values are predicted for TNT with an initial $\rho_0 = 1500$ kg/m: $p_{CL} = 19.5$ GPa, $u_p = 1.94$ km/s and $u_d = 6.70$ km/s. The predicted value of u_d is consistent with experimental results described in Ref. [6]. Figure 40 shows results from a planar **KB1** simulation for propagation of a detonation wave through a 10 cm slab of TNT (200 elements). Detonation was initiated by impact of a thin (1mm) aluminum slab moving at 5 km/s. The plot shows the pressure profile in the TNT 12.5 μs after impact. The result is in good agreement with theory. The predicted position of the detonation front is 8.38 cm.

Reference [16] describes experimental results on the variation of detonation velocity with the radius of cylindrical rods of TNT. The observed velocity in a thick rod (1.75 inch diameter) is close to the value for an infinite medium. The value for a rod of diameter 0.75 inch is lower by a factor 0.976. A **KB2** simulation with cylindrical symmetry was created to model this two-dimensional effect. The top section of Fig. 42 shows the spatial variation of pressure in the

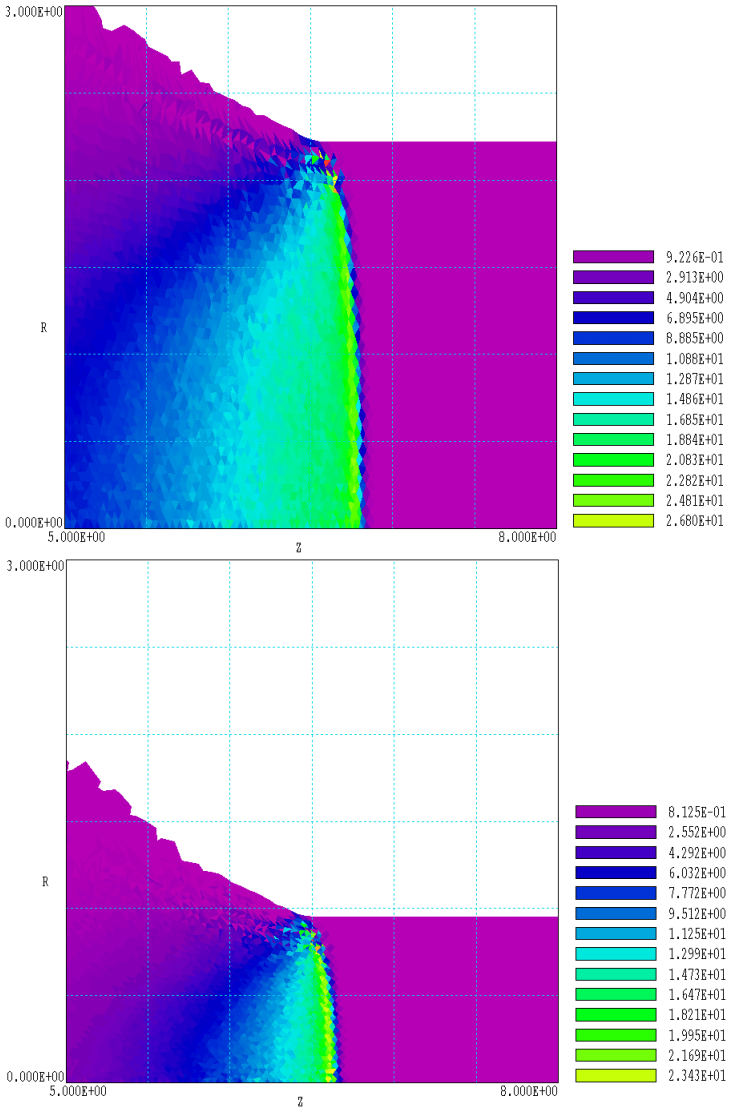

Figure 42: Pressure profiles in TNT rods at 10.0 μS, large diameter ignitor. Top: 1.75 inch diameter rod. Bottom: 0.75 inch diameter rod.

large diameter rod 10 μs after ignition. The process was initiated by a thin (1mm) aluminum plate moving at 6 km/s that struck the end of the rod ($x = 0.0$ cm) at $t = 0.0\mu$s. The plate had the same diameter as the rod to provide instantaneous ignition over the surface. In the figure note that the detonation front is very close to the predicted position of 6.7 cm. Following the Neumann spike, the pressure over the front is close to the CJ value of 19.5 GPa.In comparison, The bottom section of Fig. 42 shows the pressure profile at 10 μs in the 0.75 inch diameter rod. The difference in position caused by the small reduction in detonation velocity is clearly visible. Accurate measurements of the relative velocities were obtained by placing temporal probes near the end of the rods in the **KB2** simulations. The code gave a reduction factor of 0.974, in agreement with experiments.

To demonstrate the 2D capabilities of KB2, a simulation was created to model the growth of a detonation wave from a localized ignition point. In this case, the aluminum plate had a

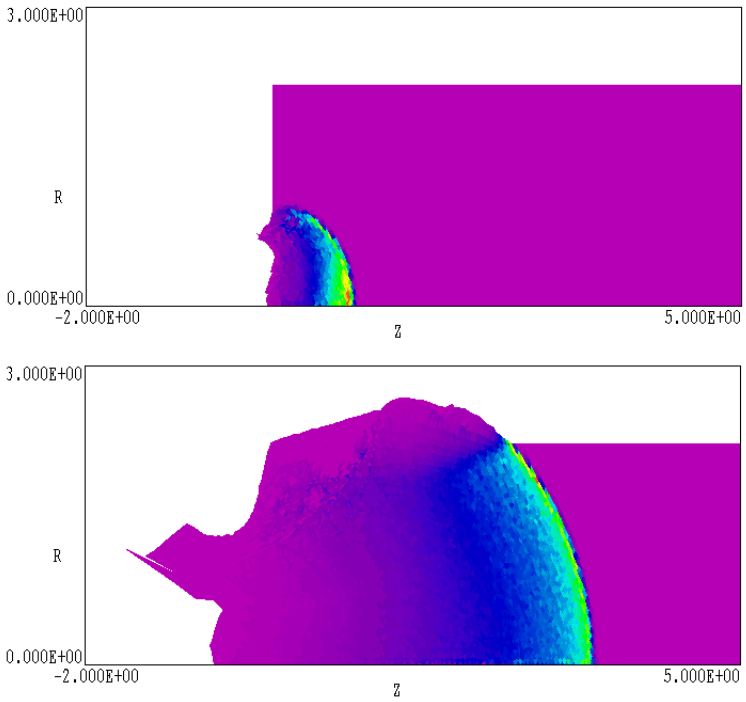

Figure 43: Pressure profile, localized ignition in a rod of TNT, 1.75 inch diameter. Top: 1.0 μs. Bottom: 5.0 μs.

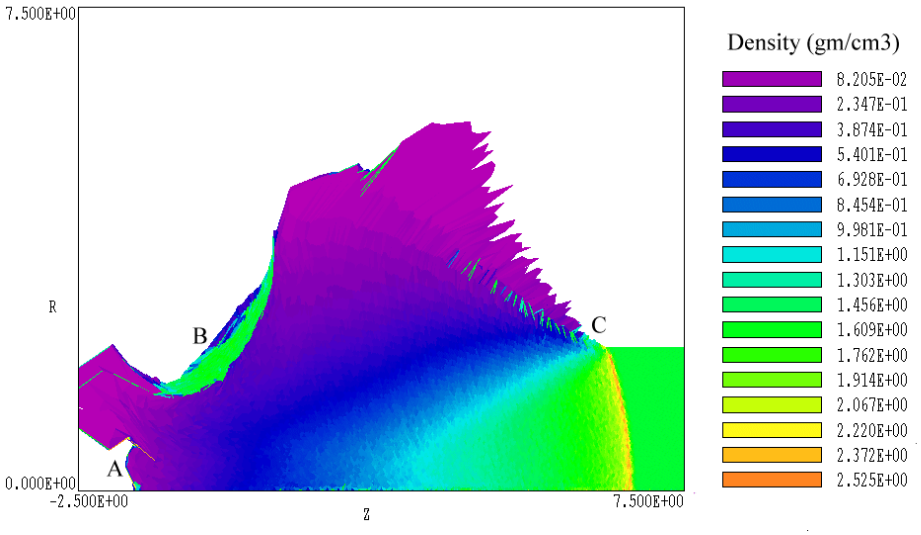

Figure 44: Density variations in a 1.75 inch diameter TNT rod with localized ignition at 10.0 μs.

radius of 0.5 cm compared to a TNT rod radius of 2.22 cm. Figure 43 shows pressure profiles at 1.0 and 5.0 μs after ignition. An approximately spherical detonation surface expands from the contact point. It maintains considerable convexity, even after reaching the outer radius of the rod (5.0 μs). Figure 44 shows density variations in the rod and blowoff plume 10 μs after ignition. The shape of the detonation front is approaching the equilibrium configuration of Figure 42. Several processes influence the shape of the plume, including the mass of the aluminum plate (A) , undetonated material from the upstream corner of the rod bypassed by the spherical front (B),and undetonated material from the thin, low-pressure region on the outside of the rod (C). The plume resembles the shapes in framing photographs of unconfined dynamite rods described in Ref. [17].

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[17] C.H.Johansson and P.A. Persson, Detonics of High Explosives (Academic Press, New York, 1970), Figure 1.6.2*a*.

Appendix: Explosive materials

The data listed is intended to give some useful parameters to model explosives in **KB1** and **KB2**, but it is by no means exhaustive. A great number of explosives have been developed with different compositions and initial densities. Here are some practical suggestions for using the data.

The shock EOS parameters are not available for most of the materials in the table. Furthermore, an inspection of entries for explosives in Ref. [13] shows that there is a considerable variation in experimental values because of the difficulty of performing the measurements. Fortunately, the characteristics of a front in fully-detonated material do not depend sensitively on the values of C_0, S_1 and S_2 used for the undetonated solid or liquid material. You can probably get acceptable results by using values for a similar non-metallic material with approximately the same initial density.

Explosives can be formulated with a broad range of initial densities. The value of Q does not depend on the initial density, but γ does. If data are not available, use the following formulas to estimate γ for a density value ρ different from the ρ_0 value in the table. The detonation velocity scales roughly as

$$\frac{u_d}{u_{d0}} \cong \left(\frac{\rho}{\rho_0}\right)^{0.6}. \tag{57}$$

The quantity γ is then given by

$$\gamma = \sqrt{1.0 - \frac{u_d^2}{2Q}}. \tag{58}$$

Explosive Material Parameters for the KB Model

Name	Density (kg/m3)	C0	S1 (m/s)	S2 (s/m)	Q (J/kg)	Gamma	PCJ (Pa)	Ud (m/s)
Ammonium picrate	1550				3.34E+06	2.83	1.90E+10	6847
Composition B	1560	2460	3.52	-8.81E-04	5.18E+06	2.63	2.63E+10	7829
Composition C-2	1570				4.68E+06	2.70	2.50E+10	7675
Composition C-3	1600				4.60E+06	2.70	2.50E+10	7605
Composition C-4	1590				5.14E+06	2.70	2.78E+10	8042
Cyclotol	1700				5.14E+06	2.69	2.95E+10	8007
DBX	1650				7.11E+06	2.02	2.39E+10	6617
Detasheet C	1450				4.14E+06	2.70	2.04E+10	7215
Dynamite (low vel)	900				2.61E+06	2.17	5.50E+09	4403
Dynamite (med vel)	1100				3.93E+06	2.36	1.18E+10	5992
EL-506D	1400				3.64E+06	2.80	1.83E+10	7054
HMX (beta)	1840	2700	2.77	-6.21E-04	5.69E+06	2.89	3.95E+10	9143
Lead azide	2000				1.55E+06	2.53	9.47E+09	4088
Lead styphnate	2900				1.92E+06	2.85	2.06E+10	5234
Mercury fulminate	2000				1.80E+06	2.10	7.91E+09	3501
Minol-2	1680				6.77E+06	1.87	1.98E+10	5815
Nitrocellulose	1200				4.43E+06	2.65	1.75E+10	7305
Nitroglycerin	1600				6.69E+06	2.33	2.85E+10	7697
Nitroguanidine	1550				3.01E+06	3.27	2.12E+10	7639
PBX-9404	1840	2621	1.70	-2.10E-05	5.50E+06	2.84	3.70E+10	8800
PBX-9010	1784	2458	2.15	-1.74E-05	5.11E+06	2.80	3.28E+10	8370
Pentolite	1660				5.10E+06	2.54	2.61E+10	7457
PETN	1700	2140	1.82	2.06E-03	5.81E+06	2.63	3.22E+10	8292
Picric acid	1710				4.18E+06	2.73	2.47E+10	7345
RDX	1650				5.35E+06	2.70	3.00E+10	8204
Tetryl	1710	2495	1.36	3.56E-05	4.60E+06	2.37	2.15E+10	6516
TNT	1500	1960	3.01	-6.02E-04	4.51E+06	2.44	1.95E+10	6684
Torpex	1810				7.52E+06	2.18	3.21E+10	7514
Tritonol	1720				7.40E+06	2.01	2.57E+10	6707

Appendix: Shock EOS parameters

The values were calculated from experimental data tabulated in S.P. Marsh (*ed.*), **LASL Shock Hugoniot Data** (University of California Press, Berkeley, 1980). A least-squares fit procedure was used to calculate the parameters C_0, S_1 and S_2. Only those materials with a sufficient number of data points were are included. The data are also available in the Excel file `shockeos.xls`. The following quantities are included in the tables:

RhoAvg: average initial density of the material in kg/m^3.

C0, S1, S2: calculated parameters

Stdv: standard deviation of experimental values of u_s from the fitted curve (m/s)

UpMax: maximum experimental value of u_p (m/s)

The parameters C_0, S_1 and S_2 can be used to find Hugoniot curves for the listed materials. The following equations [adapted from M. Meyers, **Dynamic Behavior of Materials** (Wiley, New York, 1994)] can be used to find the quantities u_p, u_s, p and ρ with internal energy U as the independent variable:

$$u_s = \sqrt{2U}. \tag{59}$$

$$u_s = C_0 + S_1\, u_p + S_2\, u_p^2. \tag{60}$$

$$p = \rho_o u_s \left(\frac{1}{2}\, u_p + \sqrt{\frac{U}{2}} \right). \tag{61}$$

$$\rho = \frac{\rho_0\, u_s}{u_s - u_p}. \tag{62}$$

The quantity ρ_0 is the density before the shock. The spreadsheet template `hugocalc.xls` apply the equations to generate a Hugoniot curve. The curve is calculated using the values supplied in the second column of the header.

Summary of Shock EOS Information

Name	RhoAvg (kg/m3)	C0 (m/s)	S1	S2 (s/m)	Stdv (m/s)	UpMax (m/s)
albitite	2.610E+03	5.468E+03	-3.800E-01	3.055E-04	1.073E+02	1.287E+03
alluvium	1.540E+03	1.584E+03	7.784E-01	1.318E-04	2.066E+02	3.993E+03
alluvium	1.800E+03	1.916E+03	7.040E-01	1.594E-04	2.717E+02	3.789E+03
aluminum	1.033E+03	5.263E+03	1.578E+00	-1.075E-04	7.520E+01	1.812E+03
aluminum	2.804E+03	5.178E+03	1.399E+00	-1.101E-05	9.140E+01	2.120E+02
aluminum	2.703E+03	5.240E+03	1.479E+00	-3.222E-05	9.991E+01	3.470E+03
aluminum	1.597E+03	1.335E+03	1.566E+00	3.497E-05	3.265E+02	3.924E+03
aluminum	1.882E+03	1.750E+03	1.745E+00	7.514E-06	3.213E+02	3.694E+03
aluminum	2.140E+03	2.475E+03	1.815E+00	-7.494E-06	2.774E+02	3.481E+03
aluminum	2.456E+03	3.849E+03	1.593E+00	2.030E-06	1.364E+02	3.233E+03
aluminum	2.784E+03	5.344E+03	1.330E+00	-8.162E-06	8.231E+01	8.420E+02
aluminum	2.828E+03	5.079E+03	1.470E+00	-2.536E-05	7.339E+01	8.620E+02
ammonia	7.260E+02	1.947E+03	1.554E+00	-6.783E-06	1.460E+02	5.310E+03
andalusite	3.074E+03	5.900E+03	6.823E-01	6.372E-05	3.400E+02	3.137E+03
anorthosite	2.732E+03	5.742E+03	-4.287E-01	3.137E-04	1.727E+02	1.272E+03
anthracene	1.249E+02	2.882E+03	1.757E+00	-1.170E-04	2.762E+02	4.810E+03
antimony	6.698E+03	2.985E+03	5.148E-01	2.814E-04	1.622E+02	2.699E+03
argon	1.650E+03	8.707E+02	2.080E+00	-9.311E-05	1.047E+02	4.600E+03
balsa	1.231E+02	2.127E+02	1.218E+00	1.557E-05	5.240E+02	7.108E+03
baratol	2.317E+03	2.385E+03	2.076E+00	-6.949E-04	1.340E+02	1.140E+03
barium	3.706E+03	1.323E+03	1.132E+00	6.881E-05	1.564E+02	3.424E+03
barium titanate	5.431E+03	2.260E+03	3.331E+00	-4.837E-04	1.205E+02	7.560E+02
benzene	8.747E+02	1.604E+03	1.704E+00	-7.473E-05	2.109E+02	1.393E+03
beryllium	1.850E+03	8.060E+03	1.042E+00	1.971E-05	6.153E+01	6.850E+02
beryllium oxide	2.528E+03	7.987E+03	-2.015E-01	4.278E-04	3.577E+02	3.034E+03
beryllium oxide	2.989E+03	9.573E+03	6.305E-01	4.630E-05	5.115E+02	2.822E+03
beryllium oxide	2.138E+03	6.263E+03	-2.498E-01	4.128E-04	2.224E+02	3.356E+03
birch	6.931E+02	2.224E+02	1.775E+00	-5.122E-05	1.686E+02	5.738E+03
bismuth	9.836E+03	1.768E+03	1.482E+00	-5.995E-06	8.670E+01	2.439E+03
boron	2.338E+03	1.030E+04	6.350E-01	-5.824E-05	3.793E+02	3.942E+03
boron carbide	2.400E+03	1.034E+04	-1.149E+00	4.683E-04	3.606E+02	1.901E+03
boron carbide	1.934E+03	1.528E+03	2.927E+00	-2.046E-04	1.596E+02	2.616E+03
boron nitride	2.145E+03	4.138E+03	2.962E-01	2.319E-04	1.616E+02	2.780E+03
boron nitride	2.082E+03	4.103E+03	-1.356E-02	3.005E-04	2.120E+02	4.264E+03
boron nitride	2.115E+03	4.028E+03	1.060E-01	2.733E-04	1.473E+02	3.589E+03
brass	8.413E+03	3.812E+03	7.748E-01	4.744E-04	1.159E+01	1.052E+03
brass	8.450E+03	3.703E+03	1.482E+00	-1.677E-05	5.192E+01	2.203E+03
bromoform	2.849E+02	2.119E+02	3.060E+00	-5.375E-04	3.071E+01	6.700E+02
bronzitite	3.296E+03	6.590E+03	-3.690E-02	2.397E-04	9.045E+01	4.850E+02
bronzitite	3.276E+03	6.379E+03	5.193E-01	8.001E-05	1.310E+02	2.096E+03
cadmium	8.639E+03	2.511E+03	1.612E+00	3.184E-06	5.408E+01	1.092E+03
calcium	1.547E+03	3.572E+03	9.784E-01	-5.972E-06	1.082E+02	4.246E+03
calcium oxide	2.980E+03	3.351E+03	2.339E+00	-2.623E-04	1.732E+02	3.010E+03
carbon	1.948E+03	3.829E+03	6.422E-01	1.213E-04	2.500E+02	2.909E+03
carbon	2.026E+03	2.543E+03	2.358E+00	-2.673E-04	1.483E+02	1.854E+03
carbon	2.134E+03	5.539E+03	-3.426E-01	3.131E-04	2.300E+02	2.779E+03
carbon	2.208E+03	4.034E+03	2.383E+00	-3.005E-04	2.470E+02	9.810E+02
carbon	2.922E+02	1.229E+03	4.204E-01	1.105E-04	1.971E+02	2.295E+03
carbon	3.150E+02	5.209E+02	1.067E+00	-1.169E-05	7.514E+01	4.631E+03
carbon	4.807E+02	4.011E+02	1.094E+00	1.225E-05	1.344E+02	4.847E+03
carbon	5.603E+02	6.333E+02	1.024E+00	2.567E-05	1.634E+02	6.271E+03
carbon	1.934E+03	5.064E+03	1.619E-01	1.345E-04	1.056E+02	3.212E+03
carbon	1.011E+03	8.246E+02	1.272E+00	4.190E-06	2.456E+02	5.395E+03
carbon	1.542E+03	7.646E+02	2.295E+00	-1.902E-04	1.165E+02	2.361E+03
carbon	1.519E+03	1.209E+03	1.857E+00	-9.177E-05	1.277E+02	9.240E+02
carbon	1.492E+03	2.961E+03	8.467E-01	4.425E-05	2.323E+02	1.741E+03
carbon	1.768E+03	2.657E+03	1.172E+00	2.636E-05	2.096E+02	4.066E+03
carbon	2.677E+02	6.976E+02	7.023E-01	8.030E-05	2.267E+02	4.793E+03
carbon	1.878E+03	2.975E+03	1.160E+00	2.993E-05	2.236E+02	2.947E+03
carbon disulfide	1.257E+03	1.706E+03	1.014E+00	3.821E-05	1.779E+02	1.362E+03
carbon tetrachloride	1.585E+03	1.059E+03	1.809E+00	-6.986E-05	1.061E+02	1.275E+03
cassiterite	6.694E+03	7.307E+03	-1.258E+00	4.457E-04	9.254E+01	2.266E+03
cellulose acetate	1.261E+03	2.081E+03	1.771E+00	-7.082E-05	1.635E+02	2.406E+03

cerium	6.743E+03	1.229E+03	1.587E+00	2.275E-05	1.435E+02	3.161E+03
cerium oxide	1.133E+03	-2.055E+02	1.447E+00	-3.345E-05	1.668E+02	3.126E+03
cesium	1.826E+03	4.171E+02	1.578E+00	-4.777E-05	1.198E+01	3.846E+03
cesium bromide	4.446E+03	1.903E+03	1.594E+00	-6.237E-05	5.766E+01	2.519E+03
cesium chloride	1.457E+03	1.470E+03	2.070E+00	-1.624E-04	2.126E+01	2.278E+03
cesium chloride	1.195E+03	1.478E+03	2.028E+00	-1.268E-04	9.825E+00	2.372E+03
cesium chloride	1.723E+03	1.482E+03	2.032E+00	-1.550E-04	2.423E+01	2.184E+03
cesium iodide	4.528E+03	1.765E+03	1.449E+00	-3.025E-05	5.414E+01	2.770E+03
cherry	5.090E+02	1.758E+02	1.619E+00	-3.835E-05	1.567E+02	6.096E+03
cherry	5.986E+02	1.378E+02	1.699E+00	-4.487E-05	1.365E+02	4.767E+03
chromium	7.119E+03	5.397E+03	1.076E+00	1.260E-04	6.540E+01	1.437E+03
cobalt	8.820E+03	4.604E+03	1.547E+00	-8.557E-05	4.943E+01	9.330E+02
composition b	1.561E+03	2.461E+03	3.517E+00	-8.810E-04	2.374E+02	6.900E+02
copper	3.832E+03	1.341E+03	7.016E-01	2.459E-04	1.068E+02	3.126E+03
copper	6.966E+03	2.397E+03	1.210E+00	1.743E-04	2.510E+02	3.063E+03
copper	5.477E+03	1.560E+03	1.087E+00	2.005E-04	2.344E+02	3.327E+03
copper	6.022E+03	1.917E+03	1.028E+00	2.123E-04	2.849E+02	3.258E+03
copper	8.924E+03	3.869E+03	1.586E+00	-2.389E-05	6.923E+01	4.840E+02
copper	4.840E+03	4.109E+03	1.431E+00	4.987E-05	1.834E+02	2.457E+03
copper	7.526E+03	2.894E+03	1.186E+00	1.805E-04	2.172E+02	2.969E+03
copper oxide	1.710E+03	2.110E+03	1.767E+00	-6.190E-05	5.654E+01	3.730E+03
corundum	3.977E+03	8.655E+03	1.080E+00	-3.101E-05	1.898E+02	2.470E+03
corundum	3.741E+03	6.935E+03	9.874E-01	8.673E-05	2.012E+02	3.118E+03
corundum	3.519E+03	7.671E+03	7.085E-01	1.617E-04	9.584E+01	2.979E+03
corundum mixture	3.389E+03	3.265E+03	2.507E+00	-1.571E-04	3.152E+01	1.728E+03
cyclohexadiene	8.470E+02	1.674E+03	1.573E+00	-3.923E-05	1.842E+02	5.400E+03
cyclohexadiene	8.400E+02	1.565E+03	1.574E+00	-3.806E-05	1.477E+02	5.430E+03
cyclohexane	7.760E+02	1.465E+03	1.789E+00	-4.367E-05	1.194E+02	5.450E+03
cyclohexene	8.100E+02	1.598E+03	1.701E+00	-4.136E-05	1.342E+02	5.270E+03
deuterium	1.650E+02	-2.398E+03	2.806E+00	-1.336E-04	2.830E+02	7.250E+03
diabase	2.987E+03	5.047E+03	4.018E-01	1.641E-04	2.065E+02	8.630E+02
diabase	3.015E+03	5.331E+03	2.349E-01	1.960E-04	1.346E+02	1.171E+03
dunite	3.240E+03	5.882E+03	1.213E+00	-7.590E-05	2.246E+02	1.454E+03
dunite	3.319E+03	6.952E+03	3.186E-01	1.070E-04	1.403E+02	1.071E+03
dunite	3.791E+03	5.994E+03	6.033E-01	6.440E-05	2.195E+02	2.914E+03
dysprosium	8.410E+03	2.264E+03	8.419E-01	9.029E-05	3.742E+01	2.670E+03
eclogite	3.551E+03	5.651E+03	1.752E+00	-1.847E-04	1.554E+02	2.491E+03
eclogite	3.418E+03	5.870E+03	1.403E+00	-1.315E-04	1.158E+02	2.599E+03
enstatite	2.950E+03	4.514E+03	1.205E+00	1.894E-05	7.749E+01	3.136E+03
enstatite	2.829E+03	3.835E+03	1.390E+00	-1.717E-06	8.451E+01	1.795E+03
enstatite	2.714E+03	1.326E+03	2.431E+00	-2.186E-04	2.565E+00	2.458E+03
enstatite	3.007E+03	5.145E+03	1.113E+00	-2.002E-05	1.466E+02	3.878E+03
epoxy	1.852E+03	3.052E+03	1.442E+00	-1.963E-05	1.343E+02	4.495E+03
epoxy	1.776E+03	2.998E+03	1.055E+00	3.373E-05	1.330E+02	1.267E+03
epoxy	2.219E+03	2.766E+03	2.105E+00	-1.072E-04	7.929E+01	5.620E+02
epoxy	2.007E+03	2.797E+03	1.949E+00	-1.059E-04	1.060E+02	4.880E+02
epoxy	2.210E+03	2.711E+03	2.050E+00	-5.942E-05	1.372E+02	6.220E+02
epoxy	2.017E+03	3.130E+03	1.582E+00	-2.773E-05	1.062E+02	3.969E+03
epoxy	2.307E+03	2.573E+03	2.164E+00	-1.009E-04	7.829E+01	2.743E+03
epoxy	1.185E+03	2.590E+03	1.681E+00	-5.983E-05	1.298E+02	3.361E+03
epoxy	2.171E+03	2.898E+03	1.874E+00	-6.160E-05	1.236E+02	5.660E+02
epoxy	1.660E+03	3.177E+03	1.073E+00	4.986E-05	1.454E+02	3.181E+03
epoxy	2.176E+03	3.645E+03	1.842E+00	-1.019E-04	1.019E+02	2.072E+03
erbium	8.348E+03	1.602E+03	1.440E+00	-6.716E-05	7.950E+01	1.073E+03
erbium	7.849E+03	1.333E+03	1.513E+00	-6.387E-05	5.485E+01	3.268E+03
erbium	9.015E+03	2.373E+03	7.217E-01	1.316E-04	5.835E+01	4.020E+02
erbium	7.169E+03	1.083E+03	1.417E+00	-3.006E-06	4.010E+01	3.333E+03
estane	1.186E+03	2.141E+03	2.117E+00	-1.586E-04	1.486E+02	5.150E+02
ethylene glycol	1.112E+03	1.877E+03	1.853E+00	-5.731E-05	1.199E+02	4.860E+03
europium	5.280E+03	1.558E+03	9.530E-01	5.616E-05	9.782E+01	8.060E+02
fayalite	4.245E+03	6.594E+03	-5.774E-01	3.453E-04	9.817E+01	1.393E+03
fir	5.361E+02	1.636E+02	1.594E+00	-3.106E-05	1.648E+02	6.056E+03
fir	3.550E+02	3.301E+01	1.546E+00	-3.341E-05	1.829E+02	6.412E+03
fkm propellant	1.610E+03	1.954E+03	2.631E+00	-2.345E-04	1.110E+02	9.020E+02
forsterite	3.105E+03	7.098E+03	7.116E-01	-3.621E-05	3.362E+02	5.120E+02
forsterite	3.059E+03	6.362E+03	-2.334E-01	2.557E-04	7.848E+01	1.779E+03
gabro	2.978E+03	6.441E+03	-1.249E+00	5.597E-04	8.444E+01	3.020E+03
gabro	2.919E+03	6.437E+03	-1.299E+00	5.539E-04	2.426E+02	3.058E+03
gadolinium	7.861E+03	2.138E+03	9.595E-01	6.433E-05	6.584E+01	2.206E+03

garnet	3.450E+03	8.118E+03	7.554E-01	-7.816E-05	3.469E+02	3.040E+03
gas shale	2.548E+03	4.360E+03	6.662E-01	1.026E-04	2.181E+02	5.270E+02
germanium	5.328E+03	3.644E+03	2.289E-01	2.838E-04	2.024E+02	1.971E+03
glass	2.230E+03	4.457E+03	-1.323E-01	2.511E-04	2.713E+02	2.397E+03
glass	5.085E+03	3.166E+03	3.510E-01	2.648E-04	1.484E+02	2.347E+03
glass	4.817E+03	3.505E+03	1.149E-01	2.993E-04	1.421E+02	2.623E+03
glycerol	1.183E+03	2.108E+03	1.959E+00	-8.119E-05	9.146E+01	2.020E+03
gold	1.924E+04	2.978E+03	1.734E+00	-8.510E-05	3.576E+01	1.724E+03
gold	1.611E+04	2.270E+03	2.132E+00	-1.473E-04	2.773E+01	1.101E+03
gold	1.554E+04	2.863E+03	1.069E+00	2.348E-04	9.686E+01	3.040E+02
gold	1.685E+04	2.848E+03	1.321E+00	1.376E-04	8.891E+01	2.900E+02
granite	2.627E+03	4.778E+03	2.854E-02	2.339E-04	1.532E+02	1.373E+03
hafnium	1.289E+04	3.084E+03	6.845E-01	1.440E-04	5.443E+01	4.390E+02
hafnium titanate	6.932E+03	2.681E+03	1.522E+00	3.104E-05	7.660E+01	3.057E+03
hafnium titanate	4.367E+03	3.364E+02	1.847E+00	-3.048E-05	5.944E+01	3.681E+03
hafnium titanate	5.597E+03	5.007E+02	2.496E+00	-1.634E-04	4.551E+01	1.791E+03
hematite	5.007E+03	6.894E+03	1.624E-01	1.104E-04	2.099E+02	2.398E+03
hmx	1.891E+03	2.700E+03	2.766E+00	-6.214E-04	1.697E+02	8.840E+02
holmium	8.734E+03	2.349E+03	7.868E-01	9.821E-05	4.430E+01	1.520E+03
ilmenite	4.787E+03	6.695E+03	-1.069E-01	2.478E-04	1.874E+02	2.608E+03
indium	7.279E+03	2.461E+03	1.534E+00	-8.883E-06	4.692E+01	1.880E+03
iridium	2.248E+04	3.779E+03	1.857E+00	-1.828E-04	6.066E+01	9.330E+02
iron	7.856E+03	3.814E+03	1.656E+00	-7.961E-06	1.100E+02	2.520E+03
iron	3.368E+03	4.106E+01	1.823E+00	-2.061E-05	1.687E+02	3.158E+03
iron	7.705E+03	4.991E+03	3.554E-01	3.277E-04	1.524E+02	4.560E+02
iron	6.647E+03	5.370E+03	1.523E+00	-6.548E-05	1.009E+02	1.411E+03
iron	4.743E+03	3.070E+02	2.315E+00	-9.945E-05	1.198E+02	2.444E+03
iron	5.627E+03	2.448E+03	8.439E-01	2.539E-04	5.071E+02	2.189E+03
iron	6.690E+03	2.903E+03	1.249E+00	1.551E-04	3.976E+02	2.049E+03
iron	7.589E+03	3.801E+03	1.798E+00	-3.046E-05	5.364E+01	2.779E+03
iron	7.175E+03	4.313E+03	1.035E+00	1.469E-04	1.464E+02	3.020E+03
iron	8.091E+03	5.044E+03	3.331E-01	3.018E-04	1.830E+02	2.801E+03
iron	7.886E+03	4.380E+03	8.930E-01	2.036E-04	1.063E+02	2.577E+03
iron	7.962E+03	4.346E+03	1.206E+00	9.620E-05	7.024E+01	2.760E+03
iron	7.652E+03	3.840E+03	1.652E+00	1.694E-05	5.223E+01	2.774E+03
iron	7.974E+03	4.256E+03	1.208E+00	9.048E-05	1.116E+02	2.777E+03
iron	7.685E+03	3.457E+03	2.007E+00	-6.295E-05	2.155E+01	2.259E+03
iron magnesium oxide	5.191E+03	4.901E+03	1.931E+00	-2.067E-04	3.242E+02	4.590E+02
jadeite	3.335E+03	6.399E+03	1.416E+00	-1.398E-04	7.037E+01	9.860E+02
kyanite	2.921E+03	8.257E+03	-2.098E+00	6.386E-04	1.300E+02	8.470E+02
lanthanum	6.138E+03	1.919E+03	1.184E+00	6.938E-05	6.908E+01	3.295E+03
lead	1.135E+04	1.984E+03	1.549E+00	-2.555E-05	4.760E+01	6.870E+02
lead zircon. titanate	7.714E+03	3.608E+03	1.476E+00	-8.115E-05	9.268E+01	4.520E+02
lithium	7.379E+02	4.213E+03	1.802E+00	-6.320E-05	8.973E+01	3.407E+03
lithium	6.650E+02	1.889E+03	2.603E+00	-1.589E-04	1.519E+02	3.526E+03
lithium	5.791E+02	9.750E+02	2.331E+00	-9.214E-05	1.121E+02	3.690E+03
lithium	5.141E+02	7.127E+02	2.160E+00	-6.329E-05	1.177E+02	3.775E+03
lithium	4.479E+02	4.671E+02	1.850E+00	-1.350E-05	9.964E+01	3.933E+03
lithium	5.300E+02	4.866E+03	9.336E-01	3.541E-05	7.617E+01	4.794E+03
lithium	7.441E+02	5.396E+03	1.346E+00	-1.311E-05	1.802E+02	5.372E+03
lithium	6.293E+02	5.896E+03	1.095E+00	3.805E-05	2.983E+02	5.484E+03
lithium	7.981E+02	6.467E+03	1.168E+00	-1.181E-05	8.926E+01	3.281E+03
lithium bromide	3.470E+03	3.116E+03	1.150E+00	3.573E-05	6.025E+01	1.948E+03
lithium chloride	2.075E+03	3.939E+03	1.395E+00	2.242E-06	5.342E+01	3.167E+03
lithium deuteride	7.929E+02	5.319E+03	1.163E+00	1.979E-05	2.167E+02	5.292E+03
lithium fluoride	2.638E+03	5.126E+03	1.384E+00	-7.149E-06	6.461E+01	6.310E+02
lithium hydride	7.265E+02	5.251E+03	1.455E+00	-2.954E-05	2.173E+02	7.590E+03
magnesium	1.776E+03	4.455E+03	1.334E+00	-2.334E-05	9.877E+01	1.990E+03
magnesium	1.105E+03	4.360E+03	1.270E+00	-4.521E-06	1.009E+02	2.348E+03
magnesium	1.740E+03	4.506E+03	1.249E+00	2.936E-06	8.023E+01	3.878E+03
magnetite	5.117E+03	6.292E+03	-1.981E-01	2.892E-04	1.701E+02	2.617E+03
mahogany	4.870E+02	-1.361E+02	1.735E+00	-4.556E-05	1.657E+02	2.190E+03
mahogany	4.120E+02	-2.285E+01	1.570E+00	-3.068E-05	1.223E+02	5.046E+03
maple	7.957E+02	4.030E+02	1.807E+00	-5.410E-05	7.526E+01	5.578E+03
melmac	1.453E+03	4.710E+03	-4.418E-01	5.385E-04	1.038E+02	1.564E+03
methane	3.325E+03	1.085E+03	1.651E+00	-7.715E-05	1.194E+02	3.930E+03
methane	1.483E+03	1.174E+03	1.724E+00	-4.967E-05	1.191E+02	4.840E+03
methane	1.325E+03	1.234E+03	1.909E+00	-9.571E-05	1.545E+02	4.710E+03
methane	2.491E+03	9.853E+02	1.805E+00	-9.352E-05	7.653E+01	4.120E+03

micarta	1.395E+03	2.190E+03	2.125E+00	-1.164E-04	1.353E+02	4.850E+03
molybdenum	1.021E+04	5.062E+03	1.353E+00	-4.777E-05	3.517E+01	9.920E+02
mullite	2.668E+03	2.181E+03	1.735E+00	-1.336E-05	1.134E+02	2.368E+03
mullite	3.154E+03	9.213E+03	-1.291E+00	3.811E-04	3.329E+01	1.042E+03
neodymium	6.980E+03	2.164E+03	6.909E-01	1.729E-04	3.623E+01	1.001E+03
neoprene	1.439E+03	1.919E+03	2.540E+00	-3.396E-04	8.222E+00	2.091E+03
n-hexane	6.570E+02	1.318E+03	1.730E+00	-3.990E-05	1.348E+02	5.670E+03
nickel	8.875E+03	4.563E+03	1.484E+00	-1.348E-05	5.306E+01	2.102E+03
niobium	8.587E+03	4.513E+03	1.104E+00	3.004E-05	3.432E+01	1.609E+03
niobium carbide	1.871E+03	1.037E+03	1.496E+00	9.748E-06	2.376E+02	2.661E+03
niobium carbide	7.232E+03	4.160E+03	2.132E+00	-1.300E-04	1.035E+02	2.825E+03
niobium carbide	7.483E+03	5.398E+03	1.434E+00	7.999E-06	1.207E+02	2.190E+03
niobium carbide	2.148E+03	9.078E+02	1.470E+00	1.714E-05	1.585E+02	2.604E+03
nitrogen	8.200E+02	9.789E+02	1.768E+00	-5.469E-05	1.356E+02	5.350E+03
nitromethane	1.125E+02	1.353E+03	2.086E+00	-1.645E-04	5.742E+01	1.841E+03
nq	1.667E+03	5.920E+03	-2.424E+00	1.304E-03	5.691E+01	1.018E+03
nq	1.699E+03	2.706E+03	2.179E+00	-1.117E-04	8.319E+01	1.744E+03
nq	1.688E+03	3.017E+03	1.763E+00	-1.082E-05	1.385E+02	1.320E+03
nq	1.717E+03	5.744E+03	-1.080E+00	7.118E-04	2.657E+02	2.072E+03
oak	5.373E+02	2.012E+02	1.623E+00	-3.469E-05	1.065E+02	2.166E+03
oil shale	2.192E+03	3.897E+03	1.033E+00	2.433E-05	1.777E+02	4.267E+03
oxygen	1.202E+03	1.080E+03	1.849E+00	-7.451E-05	6.025E+01	4.720E+03
palladium	1.199E+04	3.855E+03	1.849E+00	-1.118E-04	2.840E+01	1.399E+03
paraffin	1.920E+03	3.087E+03	1.622E+00	-1.425E-04	1.283E+02	8.470E+02
paraffin	1.662E+03	1.742E+03	2.013E+00	-1.897E-05	4.567E+01	9.320E+02
paraffin	2.073E+03	2.927E+03	2.009E+00	-1.201E-04	3.294E+01	8.170E+02
paraffin	1.736E+03	2.405E+03	1.720E+00	-2.564E-05	2.259E+01	9.010E+02
paraffin	9.173E+02	2.265E+03	2.064E+00	-8.844E-05	2.201E+02	3.947E+03
paraffin	2.353E+03	2.673E+03	2.531E+00	-1.853E-04	4.184E+01	7.780E+02
paraffin	2.198E+03	2.432E+03	2.972E+00	-3.652E-04	5.207E+01	7.920E+02
pbx	1.722E+03	2.432E+03	-6.755E-01	1.906E-03	1.702E+02	9.950E+02
pbx	1.621E+03	2.314E+03	1.928E+00	-1.040E-04	7.390E+01	3.546E+03
pbx	1.867E+03	2.621E+03	1.701E+00	-2.101E-05	6.248E+01	2.401E+03
pbx	1.761E+03	2.077E+03	3.053E+00	-8.814E-04	7.063E+01	9.320E+02
pbx	1.522E+03	2.443E+03	2.090E+00	3.076E-04	1.136E+02	6.540E+02
pbx	1.839E+03	2.846E+03	1.711E+00	-2.619E-04	1.431E+02	8.970E+02
pbx	1.779E+03	2.458E+03	2.150E+00	-1.737E-05	1.186E+02	8.970E+02
pbx	1.600E+03	1.288E+03	2.155E+00	-1.722E-04	3.693E+01	9.280E+02
periclase	2.807E+03	5.501E+03	-2.778E-01	4.469E-04	3.024E+02	2.873E+03
periclase	3.208E+03	5.325E+03	1.074E+00	1.383E-04	4.318E+02	2.851E+03
periclase	2.842E+03	8.902E+02	3.392E+00	-2.970E-04	5.127E+01	1.749E+03
periclase	3.584E+03	6.590E+03	1.433E+00	-2.477E-05	1.052E+02	1.476E+03
periclase mixture	1.693E+03	1.323E+03	1.073E+00	1.065E-04	5.101E+01	2.361E+03
periclase mixture	2.119E+03	-4.290E+02	2.803E+00	-1.723E-04	1.659E+02	2.145E+03
periclase mixture	1.577E+03	1.516E+03	9.015E-01	1.042E-04	1.952E+02	2.399E+03
periclase mixture	1.894E+03	-1.827E+02	2.887E+00	-3.377E-04	8.205E+01	2.508E+03
petn	1.600E+03	2.177E+03	-2.737E+00	7.731E-03	1.403E+02	4.800E+02
petn	1.720E+03	2.138E+03	1.819E+00	2.057E-03	2.261E+02	5.900E+02
petn	1.751E+03	2.300E+03	3.393E+00	-2.780E-03	3.317E+01	5.210E+02
petn	1.774E+03	2.546E+03	2.338E+00	-3.111E-04	1.223E+02	5.550E+02
phenanthrene	1.212E+02	2.798E+03	1.703E+00	-1.044E-04	2.864E+02	4.858E+03
phenolic	1.386E+03	2.882E+03	1.417E+00	-1.204E-05	1.775E+02	2.344E+03
phenolic refrasil	1.649E+03	3.424E+03	4.329E-01	1.463E-04	1.142E+02	1.201E+03
phenolic refrasil	1.086E+03	1.313E+03	1.393E+00	-1.035E-05	1.447E+02	4.593E+03
phenolic refrasil	1.657E+03	2.709E+03	7.912E-01	9.483E-05	1.381E+02	9.710E+02
phenolic refrasil	1.382E+03	2.151E+03	1.310E+00	6.577E-06	1.187E+02	2.583E+03
phenolic refrasil	1.651E+03	3.476E+03	4.074E-01	1.455E-04	8.506E+01	4.078E+03
phenoxy	1.181E+03	2.415E+03	1.742E+00	-7.169E-05	1.607E+02	2.413E+03
pine	4.502E+02	2.687E+02	1.467E+00	-1.894E-05	9.358E+01	6.203E+03
platinum	2.145E+04	3.619E+03	1.528E+00	-1.653E-05	8.185E+01	3.590E+03
poly 4-methyl-1-pent	8.296E+02	1.934E+03	1.737E+00	-3.647E-05	1.086E+02	3.359E+03
polyamide	1.146E+03	2.373E+03	2.069E+00	-1.208E-04	1.009E+02	2.385E+03
polycarbonate	1.193E+03	2.383E+03	1.615E+00	-6.697E-05	1.852E+02	1.279E+03
polychlorotrifluoroeth	1.981E+03	1.963E+03	1.738E+00	-2.205E-05	1.370E+02	1.130E+03
polyester	1.210E+03	2.435E+03	1.611E+00	-5.791E-05	1.762E+02	3.823E+03
polyester	1.942E+03	3.388E+03	6.102E-01	1.511E-04	5.881E+01	2.170E+03
polyethylene	9.540E+02	2.517E+03	1.879E+00	-6.121E-05	1.253E+02	2.494E+03
polyethylene	9.158E+02	2.316E+03	1.936E+00	-7.592E-05	1.121E+02	7.640E+02
polyethylene	9.540E+02	2.549E+03	1.890E+00	-6.688E-05	1.164E+02	2.493E+03

polyimide	1.414E+03	2.760E+03	1.337E+00	-2.798E-05	2.348E+02	3.286E+03
polymethylmethacrylate	1.186E+03	2.501E+03	1.673E+00	-5.485E-05	1.245E+02	4.663E+03
polyphenylquinoxaline	1.207E+03	2.612E+03	1.296E+00	-1.177E-05	2.039E+02	2.462E+03
polypropylene	9.038E+02	2.499E+03	1.793E+00	-5.738E-05	1.143E+02	2.538E+03
polystyrene	1.046E+03	2.269E+03	1.713E+00	-7.459E-05	1.833E+02	2.506E+03
polystyrene	2.857E+02	2.162E+01	1.373E+00	-1.620E-05	1.201E+02	2.301E+03
polystyrene	1.978E+02	-1.663E+02	1.330E+00	-9.507E-06	1.181E+02	2.335E+03
polystyrene	1.461E+02	1.185E+03	5.665E-01	9.048E-05	1.370E+02	2.375E+03
polystyrene	1.004E+02	-1.524E+03	1.657E+00	-2.198E-05	2.112E+02	6.953E+03
polystyrene	7.678E+01	2.190E+03	-5.183E-03	1.539E-04	1.743E+02	3.349E+03
polystyrene	5.494E+01	1.587E+02	1.036E+00	3.527E-05	4.121E+02	7.584E+03
polysulfone	1.235E+03	2.314E+03	1.621E+00	-6.285E-05	2.133E+02	2.418E+03
polytetrafluoroethyl	2.152E+03	1.404E+03	2.097E+00	-7.849E-05	8.663E+01	2.109E+03
polyurethane	3.206E+02	-1.304E+03	2.940E+00	-3.969E-04	7.149E+01	1.680E+03
polyurethane	2.803E+02	2.164E+03	1.790E-04	2.047E-04	1.293E+02	2.187E+03
polyurethane	1.593E+02	-2.754E+03	3.858E+00	-5.679E-04	6.064E+01	1.750E+03
polyurethane	1.264E+03	2.360E+03	1.780E+00	-7.554E-05	1.354E+02	4.618E+03
polyurethane	9.280E+01	-1.760E+03	3.172E+00	-4.852E-04	4.923E+01	1.772E+03
polyurethane	7.068E+02	3.269E+02	1.479E+00	-2.146E-05	1.143E+02	4.506E+03
polyvinyl chloride	1.376E+03	2.132E+03	1.651E+00	-3.402E-05	8.998E+01	3.676E+03
polyvinylidene fluor	1.767E+03	2.235E+03	1.928E+00	-8.550E-05	1.194E+02	8.160E+02
potassium	8.600E+02	2.164E+03	1.026E+00	2.720E-05	2.688E+01	4.486E+03
potassium bromide	2.750E+03	9.828E+02	2.189E+00	-1.336E-04	4.621E+01	3.492E+03
praseodymium	6.756E+03	2.039E+03	6.735E-01	2.155E-04	8.775E+01	2.291E+03
pyrene	1.275E+02	2.673E+03	1.872E+00	-1.410E-04	2.529E+02	4.497E+03
pyrolusite	4.318E+03	3.779E+03	1.449E+00	3.367E-06	1.908E+02	3.250E+03
quartz	1.450E+02	-6.073E+02	1.500E+00	1.126E-05	2.425E+02	5.267E+03
quartz	2.650E+03	4.280E+02	2.578E+00	-1.406E-04	6.643E+01	3.432E+03
quartz	1.877E+03	3.458E+03	-3.855E-02	2.250E-04	1.555E+02	4.632E+03
quartz	2.145E+03	3.566E+03	6.771E-02	2.193E-04	1.471E+02	4.474E+03
quartz	2.204E+03	5.285E+03	-7.408E-01	3.256E-04	1.899E+02	2.877E+03
rhenium	2.053E+04	3.905E+03	1.095E+00	1.522E-04	1.282E+02	2.060E+02
rhenium	2.098E+04	4.129E+03	1.573E+00	-1.482E-04	4.680E+01	9.610E+02
rhodium	1.243E+04	4.452E+03	2.008E+00	-2.345E-04	1.005E+02	1.056E+03
rubber	1.372E+03	2.186E+02	2.692E+00	-2.078E-04	1.090E+02	3.780E+03
rubidium	1.530E+03	1.504E+03	9.405E-01	6.399E-05	2.799E+01	3.967E+03
rutile	4.243E+03	7.854E+03	-1.733E-01	1.389E-04	1.745E+02	6.760E+02
samarium	7.461E+03	2.178E+03	7.298E-01	1.395E-04	5.078E+01	2.032E+03
scandium	3.195E+03	4.416E+03	8.853E-01	2.160E-06	1.040E+02	9.480E+02
serpentine	2.802E+03	6.639E+03	-4.584E-01	3.089E-04	1.056E+02	3.283E+03
silicon carbide	3.029E+03	1.024E+04	-1.937E+00	6.816E-04	1.009E+02	2.002E+03
silicon carbide	1.320E+03	6.257E+02	1.629E+00	-3.396E-05	9.626E+01	4.318E+03
silicon carbide	1.763E+03	9.276E+02	1.975E+00	-7.567E-05	1.013E+02	4.482E+03
silicon carbide	2.333E+03	-8.512E+02	4.191E+00	-4.261E-04	1.447E+02	2.517E+03
silicon carbide	3.122E+03	9.420E+03	1.347E-01	9.925E-05	4.624E+02	2.623E+03
silicon nitride	3.164E+03	8.820E+03	-6.397E-01	2.510E-04	6.867E+01	3.760E+03
sillimanite	3.127E+03	7.374E+03	-3.164E-01	2.292E-04	2.943E+02	3.099E+03
silver	1.049E+04	3.229E+03	1.598E+00	-1.407E-05	5.508E+01	2.149E+03
sodium	9.680E+02	2.770E+03	1.084E+00	2.751E-05	2.814E+01	4.309E+03
sodium chloride	9.640E+02	-2.221E+03	3.405E+00	-3.240E-04	1.744E+02	3.082E+03
sodium chloride	2.137E+03	3.500E+03	1.258E+00	1.449E-05	9.136E+01	3.940E+02
sodium chloride	2.163E+03	3.722E+03	1.037E+00	6.244E-05	1.044E+02	3.568E+03
sodium chloride	2.163E+03	3.654E+03	1.139E+00	4.207E-05	9.716E+01	4.060E+03
sodium chloride	2.165E+03	4.109E+03	7.929E-01	9.998E-05	8.649E+01	3.581E+03
sodium fluoride	2.805E+03	4.950E+03	2.851E-01	2.086E-04	1.538E+02	2.942E+03
spinel	3.278E+03	7.441E+03	9.990E-02	1.709E-04	2.151E+02	1.957E+03
spinel	3.087E+03	7.461E+03	5.901E-01	4.206E-05	2.521E+02	9.950E+02
spinel	3.622E+03	8.706E+03	-1.882E-02	1.630E-04	2.167E+02	3.033E+03
spinel	3.560E+03	7.362E+03	4.079E-01	1.301E-04	1.646E+02	3.412E+03
spinel	2.991E+03	5.484E+03	2.682E-01	2.200E-04	1.128E+02	3.124E+03
steel	8.091E+03	4.457E+03	1.080E+00	1.232E-04	1.198E+02	2.889E+03
steel	7.758E+03	4.504E+03	1.064E+00	1.272E-04	1.473E+02	2.922E+03
steel	8.129E+03	4.391E+03	1.168E+00	9.647E-05	1.007E+02	2.888E+03
steel	7.918E+03	4.489E+03	9.527E-01	1.615E-04	1.581E+02	2.921E+03
steel	7.890E+03	4.527E+03	1.575E+00	-2.770E-05	2.456E+01	2.772E+03
steel	7.910E+03	4.437E+03	1.627E+00	-4.231E-05	8.040E+01	4.480E+03
steel	7.805E+03	4.365E+03	1.173E+00	1.288E-04	1.651E+02	1.309E+03
steel	7.903E+03	4.533E+03	1.534E+00	-1.518E-05	2.726E+01	1.139E+03
strontium	2.628E+03	2.225E+03	8.109E-01	6.918E-05	1.314E+02	3.856E+03

sulfur	2.020E+03	4.191E+03	-4.457E-01	4.676E-04	8.109E+01	1.964E+03
sylgard	1.037E+03	1.272E+03	2.348E+00	-2.528E-04	1.193E+02	5.510E+02
tantalum	1.666E+04	3.394E+03	1.258E+00	-2.497E-05	2.526E+01	1.324E+03
tantalum carbide	2.054E+03	1.708E+03	1.380E+00	2.936E-06	1.084E+02	2.534E+03
tantalum carbide	1.409E+04	3.924E+03	2.015E+00	-2.174E-04	4.412E+01	1.319E+03
tantalum carbide	1.263E+04	2.693E+03	2.313E+00	-2.381E-04	1.062E+02	2.130E+03
tantalum carbide	1.860E+03	1.702E+03	5.878E-01	1.724E-04	1.534E+02	7.650E+02
tantalum carbide	1.775E+03	1.419E+03	1.658E+00	-5.821E-05	1.359E+02	8.840E+02
tantalum carbide	4.433E+03	1.082E+03	1.231E+00	9.988E-05	1.080E+02	8.090E+02
tatb	1.917E+03	3.551E+03	2.851E-01	7.747E-04	5.489E+01	1.220E+03
tatb	1.821E+03	2.326E+01	4.388E+00	-5.470E-04	5.939E+01	2.083E+03
tatb	1.912E+03	1.281E+03	3.649E+00	-5.284E-04	1.624E+02	1.532E+03
tatb	1.740E+03	1.422E+03	3.500E+00	-4.812E-04	1.982E+02	1.909E+03
tatb	1.688E+03	1.487E+03	3.692E+00	-5.822E-04	1.408E+02	1.471E+03
terbium	8.209E+03	2.185E+03	8.518E-01	9.760E-05	3.779E+01	1.562E+03
tetryl	1.700E+03	2.495E+03	1.362E+00	3.557E-05	3.953E+01	4.280E+02
tetryl	1.600E+03	1.080E+03	3.451E+00	-8.709E-04	4.967E+01	3.240E+02
tetryl	1.500E+03	2.532E+02	4.791E+00	-1.540E-03	6.380E+01	2.870E+02
tetryl	1.300E+03	-3.418E+02	4.985E+00	-1.482E-03	7.945E+01	2.960E+02
tetryl	1.400E+03	2.221E+02	4.016E+00	-9.056E-04	7.393E+01	2.970E+02
thallium	1.184E+04	1.696E+03	1.813E+00	-1.110E-04	1.106E+01	2.345E+03
thorium	1.168E+04	2.324E+03	9.704E-01	9.115E-05	3.539E+01	5.470E+02
thulium	9.291E+03	2.259E+03	8.501E-01	7.509E-05	5.350E+01	3.175E+03
tin	7.287E+03	2.611E+03	1.482E+00	1.451E-07	7.944E+01	2.859E+03
titanium	4.528E+03	5.057E+03	9.113E-01	1.986E-05	6.445E+01	5.520E+02
titanium carbide	1.480E+03	8.465E+02	1.563E+00	-2.788E-05	1.223E+02	4.576E+03
titanium carbide	2.165E+03	1.044E+03	1.830E+00	-4.186E-05	1.073E+02	4.190E+03
titanium carbide	4.450E+03	8.088E+03	-1.088E+00	4.919E-04	2.857E+02	1.498E+03
titanium diboride	4.484E+03	8.814E+03	4.720E-01	9.353E-05	1.254E+02	1.356E+03
tnt	1.491E+03	1.975E+03	3.014E+00	-6.024E-04	1.497E+02	1.790E+03
tnt	1.472E+02	3.200E+03	-2.012E-01	7.044E-04	4.117E+01	1.596E+03
toluene	8.682E+02	1.594E+03	1.793E+00	-8.532E-05	1.877E+02	1.387E+03
tourmaline	3.179E+03	7.282E+03	9.912E-02	1.300E-04	2.466E+02	3.026E+03
tuff	9.224E+02	4.367E+03	-3.615E-01	1.682E-04	1.330E+02	3.098E+03
tuff	1.695E+03	3.364E+02	2.757E+00	-2.254E-04	4.448E+02	3.937E+03
tuff	1.646E+03	1.121E+03	1.569E+00	-2.538E-05	2.338E+02	4.148E+03
tuff	1.281E+03	6.189E+02	1.555E+00	-2.631E-05	2.403E+02	4.257E+03
tuff	1.908E+03	2.508E+03	1.076E+00	8.258E-05	3.454E+02	1.726E+03
tungsten	1.381E+04	3.738E+03	1.309E+00	5.181E-05	7.688E+01	1.073E+03
tungsten	1.485E+04	3.388E+03	1.734E+00	-9.532E-05	1.212E+02	2.080E+02
tungsten	1.924E+04	4.007E+03	1.298E+00	-3.109E-05	4.542E+01	8.030E+02
tungsten	1.232E+04	3.220E+03	1.708E+00	-4.412E-05	7.766E+01	1.304E+03
tungsten	9.691E+03	2.752E+03	1.853E+00	-2.548E-05	2.002E+02	1.274E+03
tungsten carbide	1.501E+04	5.108E+03	1.408E+00	-1.261E-04	8.860E+01	4.370E+02
tungsten carbide	1.165E+04	3.999E+03	1.450E+00	2.925E-05	9.025E+01	2.160E+02
tungsten carbide	1.194E+04	3.472E+03	1.548E+00	9.046E-06	1.380E+02	1.353E+03
uranium	1.845E+04	2.574E+03	1.501E+00	1.636E-05	5.392E+01	4.260E+02
uranium	1.775E+04	-7.524E+03	1.139E+01	-2.398E-03	3.380E+01	2.436E+03
uranium	1.865E+04	-6.240E+03	1.018E+01	-2.124E-03	2.705E+01	2.382E+03
uranium	1.720E+04	2.764E+03	1.424E+00	2.604E-05	6.214E+01	1.948E+03
uranium	1.833E+04	2.689E+03	1.340E+00	6.916E-05	8.904E+01	2.151E+03
uranium	1.883E+04	2.459E+03	1.650E+00	-5.297E-05	3.631E+01	2.261E+03
uranium	1.893E+04	2.481E+03	1.559E+00	-1.592E-05	1.005E+02	3.463E+03
uranium	1.741E+04	2.589E+03	1.454E+00	4.206E-05	3.073E+01	2.093E+03
uranium	1.765E+04	-7.192E+03	1.092E+01	-2.257E-03	3.005E+01	2.434E+03
uranium	1.731E+04	2.697E+03	1.425E+00	3.357E-05	3.515E+01	9.540E+02
uranium	1.858E+04	-4.996E+03	9.159E+00	-1.916E-03	4.079E+01	2.385E+03
uranium dioxide	1.034E+04	3.975E+03	1.679E-01	3.017E-04	6.929E+01	1.658E+03
uranium dioxide	6.347E+03	1.850E+01	2.145E+00	-1.061E-04	8.184E+01	2.285E+03
uranium dioxide	4.306E+03	1.294E+02	1.507E+00	1.050E-06	1.311E+02	1.476E+03
uranium dioxide	3.111E+03	-1.534E+02	1.418E+00	8.978E-06	1.024E+02	3.023E+03
uranium hydride	1.092E+04	2.104E+03	1.480E+00	-2.071E-04	6.672E+01	6.820E+02
vanadium	6.099E+03	5.230E+03	9.461E-01	7.603E-05	5.732E+01	2.464E+03
vop-7 propellant	1.738E+03	2.405E+03	2.078E+00	-1.728E-04	1.356E+02	1.157E+03
walnut	6.323E+02	2.708E+02	1.694E+00	-4.582E-05	1.484E+02	2.143E+03
water	9.982E+02	1.506E+03	1.999E+00	-1.049E-04	5.312E+01	2.530E+03
wollastonite	2.822E+03	7.280E+03	-1.686E+00	5.772E-04	8.651E+01	2.090E+03
wollastonite	2.565E+03	5.388E+03	6.199E-01	3.864E-05	2.154E+02	3.282E+03
xtx	1.530E+03	1.401E+03	3.657E+00	-3.342E-04	1.608E+02	7.800E+02

ytterbium	7.019E+03	1.354E+03	9.634E-01	8.947E-05	7.055E+01	4.880E+02
yttrium	4.579E+03	3.403E+03	5.827E-01	1.383E-04	5.648E+01	1.681E+03
zinc	7.139E+03	3.107E+03	1.418E+00	4.077E-05	5.090E+01	2.663E+03
zinc chloride	1.711E+03	1.589E+03	1.977E+00	-1.059E-04	1.457E+01	2.188E+03
zinc chloride	1.475E+03	1.567E+03	2.039E+00	-1.323E-04	2.718E+01	2.270E+03
zinc chloride	1.309E+03	1.544E+03	2.069E+00	-1.426E-04	1.945E+01	2.343E+03
zirconium	6.506E+03	3.920E+03	6.265E-01	1.546E-04	4.910E+01	5.360E+02
zirconium diboride	5.992E+03	6.575E+03	4.370E-01	2.077E-04	1.498E+02	2.758E+03
zirconium dioxide	4.089E+03	4.407E+03	-3.524E-01	4.780E-04	2.217E+02	1.736E+03

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