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T. M. GRACE, N. T. SHIANG, AND J. R. HOPENFELD

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Energy Conversion and Scaling Rules for Steam Explosions

T. M. Grace and N. T. Shiang
The Institute of Paper Chemistry
Appleton, Wisconsin

and

J. R. Hopenfeld
Nuclear Energy Commission
Washington, D.C.

ABSTRACT

Energy conversion efficiencies, thermal to mechanical, for smelt-water explosions in recovery boilers are compared to thermodynamic efficiencies and to efficiencies obtained in various steam explosion experiments. Global efficiencies for smelt-water explosions are only about 0.1 to 1% of the thermodynamic efficiencies, about one order of magnitude lower than efficiencies obtained with other intermediate scale systems. Smelt-water explosion efficiencies calculated on a "localized" basis range from 1 to 20% of the thermodynamic efficiencies, similar to other intermediate scale systems. A simplified engineering analysis of explosion energetics is developed to help interpret the data and to provide a basis for estimating the effects of size scale. The analysis suggests that global energy conversion efficiencies should decrease as the size of the system increases.

INTRODUCTION

Violent explosions can take place when two liquids are brought into direct contact and the temperature of the hot fluid is well above the boiling temperature of the cold fluid. When the cold fluid is water, these explosions are usually referred to as steam explosions. These explosions are noncombustible in nature and involve the sudden, violent generation of steam (vapor). Explosions of this type have been encountered in the kraft paper industry, the steel and aluminum industries, and the liquefied natural gas industry and are considered in the analysis of hypothetical accidents in the nuclear power industry.

Steam explosions are still not very well understood. Extensive effort has been devoted to identifying the necessary conditions for such explosions, the probability of occurrence, the pressure-time characteristics, and the mechanical energy in the blast wave. It is now generally accepted that explosions proceed through four stages: coarse mixing, in which the two fluids are kept apart by a vapor film; triggering, in which a local shock wave develops which collapses the vapor film separating the fluids; escalation, in which the propagating shock wave fragments the coarse mixture, resulting in very large contact areas, rapid heat transfer, and vaporization at an explosive rate; and expansion and destructive work. Complex, highly-detailed models of aspects of this phenomenon have been developed, but they have not resulted in a predictive capability for any industrially important condition.

One of the critical issues concerning steam explosions is the estimation of the fraction of the thermal energy of the hot fluid that is converted into mechanical energy (work) during the explosion. Much experimental work involving different fluid-pairs, different contact methods, and different size scales has

been undertaken to resolve this question. Analyses of the damage patterns from a few industrial accidents have been carried out to provide additional information. The results have been confusing. Energy conversion efficiencies range from 0.001 to 10% of the available thermal energy, and there is no clear pattern as to what governs the efficiency.

Steam explosions occur in the kraft paper industry. During processing of spent pulping liquor for chemical recovery, the concentrated liquor is burnt in a recovery boiler producing a mixture of molten sodium carbonate and sodium sulfide (smelt) which collects on the hearth and is then drained out and dissolved in water. Steam explosions have occurred within the recovery boiler as well as in the dissolving tank. Information on smelt-water explosions in recovery boilers has been accumulated and provides a data base for estimating energy conversion efficiencies in large scale systems. A study of the energetics of smelt-water explosions has provided energy conversion efficiencies for 19 incidents (NUREG/CR-4745) (1). Structural models for recovery boilers and dissolving tanks were developed and used to calculate the amount of mechanical energy consistent with the observed damage. These data, along with estimates of the amount of smelt and water, were used to calculate the energy conversion efficiencies of the explosions. The calculated efficiencies were all extremely low, ranging from 0.005 to 0.37%. These results raised the question as to whether the low efficiencies were just a characteristic of the smelt-water system, or if they are a general characteristic of large scale systems.

In dealing with this issue, one is forced to deal with the broader question of how to "scale" data for these types of explosions. This might be stated as finding means to project the degree of violence observed in small laboratory tests, involving small masses of fluids, to industrial scale installations where

the masses are three to four orders of magnitude larger. More broadly, the question is one of determining how to use yield and pressure data obtained for one fluid-pair at one size-scale to predict what would happen with another fluid-pair at another size-scale.

A complete, quantitative answer to the scaling question is beyond the scope of this paper. Instead we will seek to formulate a simple scaling criterion and to determine the conditions when it can be applied. The heart of the approach is a focus on energy rather than other characteristics of the explosion.

ENERGY CONVERSION EFFICIENCIES

Thermodynamic Efficiency Calculations

Steam explosions involve the conversion of a portion of the thermal energy in the hot fluid into work or mechanical energy. Since heat energy is being converted into work, the second law of thermodynamics places an upper bound on the energy conversion. The maximum conversion efficiency can be calculated by devising reversible paths for carrying out the interaction and making an appropriate calculation of the work done.

Thermodynamic energy conversion efficiency calculations usually follow an approach first described by Hicks and Menzies (2). The interaction is assumed to take place as a two-step process in a closed system. The first step is a constant volume heat transfer between the two fluids (e.g., smelt and water) without vaporization until a single intermediate "equilibrium" temperature is reached. Step two is a reversible adiabatic expansion to ambient pressure with both fluids remaining in thermodynamic equilibrium with each other throughout the expansion. An alternative and more realistic second step is an isentropic expansion of the coolant (water).

We have modified the Hicks-Menzies approach slightly. The intermediate equilibrium temperature is based on constant specific heat of the hot fluid and no phase changes. The coolant state is assumed to be on the saturation line for pressures below the critical pressure and to extend along the critical pressure line for temperatures above critical. The expansion step is taken as an isentropic expansion of the coolant (water) only.

The calculation is straightforward. The intermediate equilibrium temperature is calculated from the masses, specific heats and temperatures of the two fluids according to the equation,

$$T_e = (M_H * C_{VH} * T_H + M_C * C_{VC} * T_C) / (M_H * C_{VH} + M_C * C_{VC}) \quad (1)$$

For equilibrium temperatures near or above the critical value, a trial and error procedure is necessary, since the specific heat of the coolant (water) is not constant.

For a closed process, the work done during the isentropic expansion is equal to the internal energy change in going from the intermediate "equilibrium" temperature to that corresponding to ambient pressure. Steam Tables (3) are used to carry out this calculation. The reference temperature for the thermal energy is taken to be the boiling point of water, 100°C.

Plots of the thermodynamic energy conversion efficiency for the smelt-water system are given in Figure 1. The main parameter influencing the efficiency is the relative mass of water and smelt. Smelt temperature has only a minor effect on efficiency because of the low specific heat of smelt. Water temperature has a greater influence. The highest efficiencies are obtained at intermediate mass ratios with the efficiency dropping off at both low and high water/smelt ratios.

At low water/smelt ratios the intermediate "equilibrium" temperature will approach the smelt temperature and the specific internal energy change during the expansion will be greatest, but the total work done is small because this internal energy change will be multiplied by a small mass of water. Explosive violence at this end is limited by the amount of water. At high water/smelt ratios the intermediate temperature will be low so the specific internal energy of the coolant before expansion will be low. This effect is magnified if the original water temperature is substantially below the boiling point. At the extreme, the intermediate "equilibrium" temperature will be below the boiling point at ambient pressure and the work obtained by expansion will be negligible. In this case the explosion is quenched by overwhelming the smelt with water. (Note, this is what normally takes place in a smelt dissolving tank.)

(Figure 1 here)

A comparison between the thermodynamic energy conversion efficiency for smelt-water and that for thermite-water is given in Figure 2. The shapes of the curves are very similar. Thermite-water shows a higher peak efficiency because thermite has a much higher temperature and only slightly smaller heat capacity than smelt. The maximum occurs at coolant/melt mass ratios of 0.63 for smelt and 1.3 for thermite. The thermite-water efficiency can be as much as 40% greater than that for smelt-water, but there is little difference for mass ratios below about 0.2.

The base for these efficiencies is the heat in the hot fluid referenced to the boiling temperature of the coolant at ambient conditions (373°K for water). This is the most logical basis to use.

Actual Energy Conversion Efficiency

The thermodynamic efficiency determines the maximum amount of work which could be obtained. In any real system the work would be less. Conceptually, one can look upon the deviation between the actual work and the thermodynamic work as resulting from an inability of the two fluids to completely intermix and exchange heat within the time scale of the explosive interaction. This can be treated quantitatively by introducing a mixing parameter, F, in conjunction with the thermodynamic efficiency, e. The mechanical energy or explosion yield is then given by

$$E = Q * e * F \quad (2)$$

where, E = mechanical energy (work) from the explosion

Q = thermal energy available in the hot fluid

e = maximum energy conversion efficiency from thermodynamics

F = fraction of the system that mixes to an extent that the thermodynamically calculated amount of work is obtained.

The remainder of the system, (1-F), is assumed to do no work.

NOTE: The reference temperature for the thermal energy, Q, must be the same as that used in the thermodynamic analysis for calculating e.

The thermal energy of the hot fluid is given by the product of the mass, the specific heat, and the difference between the hot fluid temperature and the reference temperature.

$$Q = M_h * C_{ph} * (T_h - T_r) \quad (3)$$

The thermodynamic efficiency is a function only of the temperatures of the hot and cold fluids, the reference temperature chosen, the cold to hot fluid mass

ratio, and the properties of the two fluids. It is not a function of any parameter having to do with the size scale of the system.

$$e = e(T_h, T_c, T_r, M_c/M_h, \text{properties}) \quad (4)$$

The actual energy conversion efficiency is given by E/Q . Thus data on the mixing parameter can be obtained by measuring the explosive work and dividing it by the thermal energy and the thermodynamic efficiency.

$$F = (E/Q)/e \quad (5)$$

This is considered in the next section.

Energy Conversion Efficiency Data Industrial Scale

A study of the energetics of smelt-water explosions has provided energy conversion efficiencies for 19 incidents, 18 recovery boiler explosions and one dissolving tank explosion. Efficiencies were calculated as the ratio of the mechanical deformation energy to the total thermal energy in the smelt. Details are given in NUREG/CR-4745 (1). The energy conversion efficiencies for these 19 incidents are summarized in Table 1. Thermodynamic efficiencies are provided for comparison along with calculated values of the mixing parameter.

(Table 1 here)

The energy conversion efficiencies for the smelt-water explosions are very low. The highest value was 0.37%. Only four other explosions had efficiencies greater than 0.1%. The ratio of the actual efficiencies to the thermodynamic efficiencies ranged from 0.03% to about 5%. The dissolving tank case (DT) is interesting in that an explosion occurred even though the thermodynamic analysis indicates there would be no work done on a global basis. In this case the

inefficiency of the mixing process led to the explosion. This illustrates a weakness in an analysis based on a single mixing parameter.

One obvious reason for the very low energy conversion efficiencies in the recovery boiler explosions was that not all of the smelt within the furnace was involved in the explosive interaction. The molten smelt is present on the hearth of the furnace along with solidified smelt and unburned char. Furnace dimensions are on the order of 20 to 40 ft square, and the molten smelt inventory, even though it is many tons, corresponds to an average smelt depth of only a few inches. When water enters the furnace cavity from some source, it is unlikely that it would uniformly contact all of the smelt. In some of the incidents there is clear evidence in the form of localized indentations of the floor that only a part of the smelt took part in the interaction. For these incidents it is possible to calculate a localized energy conversion efficiency, based only on the amount of smelt in the interaction area, and to compare it with the thermodynamic conversion efficiency. The results of such a comparison are shown in Table 2. The area fraction given is the indented area over the total floor area. The local efficiency is obtained by dividing the deformation energy by the product of the total thermal energy and the area fraction. The localized energy conversion efficiencies are about 1-20% of the thermodynamic efficiencies.

(Table 2 here)

Laboratory Scale

Anderson and Bova (4) reported the measured work was 35% of the isentropic coolant expansion work for small scale experiments with molten NaCl and water. These experiments were carried out with very low coolant/melt mass ratios. Their calculation of the isentropic work was based on the coolant (water) heated

to the melt temperature instead of the heat in the molten salt. The actual energy conversion efficiency ranged from 0.006 to 0.025%. Later, Anderson and Armstrong (5) investigated small-scale aluminum-water explosions using several different contacting techniques. They found explosion yields as high as 62.5% of the isentropic coolant expansion work.

Table 2. Localized explosion energy conversion efficiencies.

Incident Number	Thermal Energy, 10^6 Btu	Mechanical Energy, 10^3 Btu	Area Fraction	Local Efficiency, %	Thermodynamic Efficiency, %	Efficiency Ratio, %
6	10.3	5.2	1/25	1.26	20.5	6.1
10	26.5	28.0	1/6	0.63	3.5	18.
27	17.9	14.0	1/3.7	0.29	9.1	3.2
37	7.9	6.6	1/2	0.17	< 21.5	> 0.8
43	11.2	14.0	1/4	0.50	20.	2.5
45	14.7	4.5	1/6	0.18	19.	0.95
48	10.4	5.3	1/3.3	0.17	19.	0.90

Bergman and Laufke (6) reported a "TNT equivalent" ranging from 0.03 to 0.2 for experiments in which a small amount of water (10-100 g) was introduced into a large amount of smelt (10-30 kg) at 900°C. "TNT equivalent" is an energy unit corresponding to about 2 MJ/lb (1) or about 4400 kJ/kg (1840 Btu/lb). The isentropic coolant expansion work for this case (water expanding from 900°C) is 1330 kJ/kg. A "TNT equivalent" of 0.2 amounts to 880 kJ/kg which is 66% of the isentropic work. This is greater than the 35% found by Anderson and Bova (4), and close to the 62.5% found by Anderson and Armstrong (5).

These data indicate that systems in which a small amount of coolant is effectively dispersed in a large amount of melt can approach thermodynamic bounds.

The only experiments that yielded a high % of the thermodynamic work involved small amounts of water dispersed in large quantities of melt. Such a contact geometry is conducive to getting the most possible work out of a limited amount of water, but it does not lead to highly energetic events and it does not simulate industrially important situations. The most dangerous situations have mass ratios close to the peak in the efficiency curve, since this results in the greatest amount of mechanical work being obtained.

Intermediate Scale

Intermediate scale experiments with thermite-water were performed by Buxton and Benedick (7) in an open system. They measured the mechanical energy in crushing aluminum honeycomb blocks beneath the interaction vessel and the plastic work done in deforming the interaction vessel, and used high speed motion pictures to measure the kinetic energy of the ejecta. They did not measure the mechanical energy in the shock wave leaving the top of the interaction vessel. The highest value of the conversion efficiency that they found was 1.34% of the thermal energy of the thermite. Most values were between 0.1 and 1.0%.

Mitchell and Evans (8) performed a series of experiments in which 18.7 lb of thermite was delivered into a water mass 1.5 to 15 times greater in a closed container. They measured the kinetic energy in the water slug by a combination of high speed motion pictures and fast response pressure gages as well as the energy in pressurizing the chamber air. They found the kinetic energy ranged between 0.3 and 1.6% of the thermal energy in the thermite while the energy in pressurizing the chamber air ranged between 0.2 and 8.6% of the thermal energy in the thermite. It was later shown by Baker (9) that only a portion of the pressure energy stored in the chamber could do work on the surroundings. After

applying the necessary correction, the maximum energy conversion efficiency in these experiments decreased from 9.9 to 4.7%

Corradini et al. (10) later reported that the conversion ratio for the experiments done at Sandia were consistently in the 1-2% range. High pressure peaks (10-30 MPa) are measured near the leading edge of the explosion wave propagating at velocities of 200-600 m/sec through the mixture. Lower sustained pressures follow behind the peak.

While data are not provided on the thermodynamic efficiencies for the above experiments, the thermodynamic efficiencies for thermite and water are between 15 and 30% over a wide range of coolant/melt ratios. Thus the ratio of actual efficiency to thermodynamic efficiency ranges between about 1 and 10% for these cases.

Other Systems

Kottowski et al. (11) carried out a series of experiments with controlled fine fragmentation and mixing. Both stainless steel and uranium dioxide granules, 200 micrometers in diameter, were heated to sintering temperature and then subjected to the impact of a high pressure water column in a shock tube. Explosions occurred at an impact pressure greater than 1 mPa for the stainless steel and at impact pressures greater than 2.6 mPa for UO₂. The mechanical work was calculated from pressure and vapor void recordings from consecutive time steps. The energy conversion ratios scatter between 0 and 3%.

Bird (12) investigated the thermal interaction between 0.5 kg of molten uranium oxide at 3600°K and 55 liters of water. The energy conversion ratios were calculated on the basis that only fragmented material with particle size less than 280 micrometers was involved in the interaction. He reported the average conversion efficiencies in the restricted release and free release mode

were 6.8 and 3.2% of the Hicks-Menzies value (750 kJ/kg), respectively. (While not specifically stated, the Hicks-Menzies value of 750 kJ/kg is probably the thermodynamic work, assuming complete equilibrium between melt and coolant during the expansion. The more realistic, isentropic expansion of the coolant which we use would give a value about half as much.) The maximum conversion found by Bird was about 13% of the Hick-Menzies value. This is estimated to be about 6.5% of the thermal energy in a small fraction (about 6% of the total charge) of material actually involved in the explosion. The overall energy conversion efficiency for this case would be about 0.4%.

Summary of Experimental Data

Smelt-water explosions in recovery boilers were extremely inefficient, involving only 0.005 to 0.37% of the thermal energy in the melt. The efficiencies were only 0.03% to about 5% of the thermodynamic efficiencies. In only three cases was the energy conversion efficiency over 1% of the thermodynamic efficiency. One reason for this behavior is that one of the characteristic dimensions of the smelt pool is between one to two orders of magnitude smaller than the other two dimensions. For those few cases where the damage pattern was sufficient to define a localized interaction area, localized energy conversion efficiencies ranged from about 1 to 20% of the thermodynamic efficiencies. Thus the inhomogeneous distribution of the smelt within the furnace seems to be responsible for at least one order of magnitude of the low efficiency. This suggests that the size scale of an interaction may be determined by the smallest characteristic dimension of the system.

Laboratory scale experiments at very low coolant/melt ratios with effective dispersal techniques can give interactions in which the actual work approaches the maximum thermodynamic work. In this case, however, the maximum work is a very small fraction of the available thermal energy, so these interactions are not very energetic.

Intermediate scale experiments with thermite/water gave energy conversion efficiencies which were about 1-10% of the thermodynamic efficiency. Confinement tended to give somewhat higher efficiencies.

Kottowski's (11) experiments with hot granular material gave efficiencies of up to 15% of the thermodynamic efficiency. This indicates that a mixing inefficiency on the order of one magnitude exists even after the material has been fragmented to a size scale of about 200 micrometers. Bird's (12) data are similar. Energy conversion efficiencies were on the order of 10% of the thermodynamic efficiency (isentropic expansion of coolant) even though they were based only on the material that was smaller than 280 micrometers.

ENGINEERING ANALYSIS OF MIXING

The mixing parameter, F , would be a function of melt and coolant temperatures, mass ratio, properties, system geometry and size, contact method and triggering action. The scaling question reduces to being able to predict how F depends on these variables, since Q and e are directly calculatable for any system. A complete, quantitative, predictive function for F is not attainable. In reality, F is a probability distribution function, as is evident from the fact that macroscopically similar situations result in a broad range of explosive yields. We will have to be content with developing scaling criteria which govern the range of F .

The experimental data on energy conversion efficiency are summarized below. The objective of the engineering analysis is to provide a basis for understanding this experience.

1. If $M_c \ll M_h$, and dispersal is effective; $F \rightarrow 1$ while $e \rightarrow 0$.

Very little work is done.

2. If M_c and M_h are the same order of magnitude, and system dimensions are homogeneous; F is in the range of 0.01 and 0.1.
3. If M_c and M_h are the same order of magnitude, and one system dimension is much smaller than the others; F is about one order of magnitude smaller than it would be if all system dimensions were homogeneous.
- 4a. If $M_h \ll M_c$, dispersal is effective, and the coolant is at saturation temperature; $F \rightarrow 1$ and $e \rightarrow$ constant value, but the work, E , will be small because Q is very small.
- 4b. If $M_h \ll M_c$, dispersal is effective, and the coolant temperature is below saturation; $F \rightarrow 1$ while $e \rightarrow 0$. Little or no work is done.
- 4c. If $M_h \ll M_c$, the coolant temperature is below saturation, and the coolant is not completely mixed; work could be done even if $e = 0$. The quench action of the coolant would not be complete. This does happen in dissolving tank explosions.

It is evident that a single mixing parameter cannot be used to describe explosion energetics over the full range of coolant/melt mass ratios. This is especially so with very high coolant/melt ratios and some subcooling, where the thermodynamic efficiency is zero on a global basis. In this case it is only the inefficiency of the mixing process that results in an explosive interaction. This cannot be handled with a single parameter because F would have to approach infinity as e went to zero in order to get a finite amount of work. This doesn't fit with the concept of a mixing parameter, which assumes thermodynamic efficiencies in a fully-mixed system as an upper bound.

A better approach is to define separate mixing parameters for the hot and cold fluids, f_h and f_c . Then the masses of fluids which interact (to the thermodynamic limit) are $f_h * M_h$ and $f_c * M_c$, respectively. The thermal energy available is then given by

$$Q_a = f_h * M_h * C_{ph} * (T_h - T_c) = f_h * Q \quad (5)$$

The thermodynamic efficiency would then be given by

$$e' = e' [(f_c/f_h) * (M_c/M_h), T_h, T_c, T_r, \text{properties}] \quad (6)$$

In general, e' is a highly nonlinear function of the mass ratio and hence of the ratio of the mixing parameters. The work done, E , is given by

$$E = f_h * Q * e' = F * Q * e \quad (7)$$

Thus the measured efficiency parameter, F , can be expressed as

$$F = f_h * e' / e \quad (8)$$

It should be noted that the only variable that causes e' to differ from e is the mass ratio which is $(f_c/f_h) (M_c/M_h)$ for e' and (M_c/M_h) for e . All other variables are the same. Thus $e' \approx e$ when $(f_c/f_h) \approx 1$ or if the mass ratio is in the range where the thermodynamic efficiency is not a strong function of the mass ratio. The greatest differences between e and e' are expected at the extremes ($M_c \ll M_h$ or $M_h \ll M_c$). In the intermediate range the efficiency is relatively independent of the coolant/melt ratio and so $e' \approx e$ and $F \approx f_h$.

Thermodynamic efficiencies are calculated by a two-step process.

1. The system attains an "equilibrium temperature," T_e , which is determined by a simple heat balance.

$$T_e = \frac{M_h * C_{ch} * T_h + M_c * C_{vc} * T_c}{M_h * C_{vh} + M_c * C_{vc}} \quad (9)$$

where the C_v 's are appropriate averages over the temperature interval.

Thus $T_e = T_e (T_h, T_c, M_c/M_h, \text{properties})$ and is bounded, $T_c < T_e < T_h$.

2. The work is obtained by an isentropic expansion of the coolant from T_e down to the temperature corresponding to the reference pressure, P_r (normally ambient pressure). Then the work per unit mass of coolant, w , is given by $w = w (T_e, P_r, \text{coolant properties only})$, with $w = 0$ if $T_e < T_{\text{sat}}$ (at P_r).

The two extreme cases can now be analyzed.

Water Limited Case

If $M_c \ll M_h$, then $T_e \rightarrow T_h$, and $w = w (T_h, P_r, \text{coolant properties})$. The thermodynamic efficiency is then given by

$$e = \frac{M_c * w (T_h, P_r, \text{coolant properties})}{M_h * C_{ph} * (T_h - T_r)} \quad (10)$$

Thus e is a linear function of the coolant/melt mass ratio at low values of that ratio.

For the case with two mixing parameters, the interactive efficiency, e' , is given by

$$e' = \frac{f_c * M_c * w (T_h, P_r, \text{coolant properties})}{f_h * M_h * C_{ph} * (T_h - T_r)} = \frac{f_c * e}{f_h} \quad (11)$$

Combining Eq. (11) with Eq. (8) gives

$$F = f_c \text{ for } M_c \ll M_h \quad (12)$$

Thus for the water limited case, the thermodynamic efficiency is directly proportional to the coolant/melt mass ratio and the water mixing parameter is the only significant mixing parameter. The experimental data indicate that f_c can approach unity when $M_c \ll M_h$ under some conditions.

Melt Limited Case

The situation of primary interest here is that of poor mixing. In this case the amounts of each fluid which interact are given by $f_c * M_c$ and $f_h * M_h$.

$$T_e = \frac{f_c * M_c * C_{vc} * T_c + f_h * M_h * C_{vh} * T_h}{f_c * M_c * C_{vc} + f_h * M_h * C_{vh}} \quad (13)$$

$$\text{or } T_e \approx T_c + (f_h/f_c) * (M_h/M_c) * (C_{vh}/C_{vc}) * T_h \quad \text{for } M_h \ll M_c \quad (14)$$

No work is done if $T_e < T_{sat}$, and this occurs if $(f_h/f_c) * (M_h/M_c) \rightarrow 0$ and $T_c < T_{sat}$. If $T_c > T_{sat}$, there will be a finite amount of work which will tend to be proportional to $(f_h/f_c) * (M_h/M_c)$.

The global equilibrium temperature is given by

$$T_e = \frac{T_c + (M_h/M_c) * (C_{vh}/C_{vc}) * T_h}{1 + (M_h/M_c) * (C_{vh}/C_{vc})} \quad (15)$$

Comparing Eq. (14) and (15), it can be seen that when $T_c < T_{sat}$, it is possible for T_e (global) $< T_{sat}$ while T_e (interactive) $> T_{sat}$, if f_h/f_c is sufficiently greater than 1. This would occur if $f_h \rightarrow 1$ while $f_c \ll 1$, which is what happens in a dissolving tank explosion.

Intermediate Region

The region of greatest interest is that of intermediate mass ratios where the magnitude of the thermodynamic efficiency is highest and is also relatively independent of mass ratio. In this region, $F \approx f_h$, and we can focus on the mixing of the hot fluid.

The first case to be considered is one where the two fluids are uniformly intermixed on a coarse scale and the system is dimensionally homogeneous (each spatial dimension is approximately the same). We will formulate a simple analysis of this case and then extend it to more complex situations.

The conceptual model used to formulate the analysis considers that the explosion initiates at a triggering point. The disturbance then propagates through the mixture causing mixing, rapid heat transfer, and violent expansion. Mixing and thermal interaction are assumed to occur first. The expansion which follows is assumed to terminate the mixing process. In any local region, there will be a characteristic interaction time interval, t_i , from the start of the rapid mixing process until the start of expansion. If the disturbance propagates at a velocity, c , there will also be a characteristic interaction length, L_i , given by $L_i = c \cdot t_i$. These two parameters, t_i and L_i , can be used to derive scaling relationships. Mechanical constraints placed on the system will tend to delay the start of expansion and this will result in an increase in t_i and thus L_i .

One of the critical aspects of steam explosions is that of coherency. An energetic explosion can only occur if the mixing and thermal energy transfer takes place in a coordinated manner within the time scale of the explosion. This effect must be incorporated into the "mixing model." This can be done by writing the hot fluid mixing function, f_h , as a product of a coherency factor, f_{coh} , and a mixing/heat transfer factor, f_{mix} .

$$f_h = f_{coh} * f_{mix} \quad (16)$$

The coherency factor accounts for the fraction of the global system volume that is able to participate in the coordinated interaction, while the mixing/heat transfer factor accounts for the local processes that allow extremely rapid energy transfer to the coolant.

The mixing factor, f_{mix} , involves two separate but interlinked physical processes, the increase in the thermal contact area, A_h , as the two fluids intermix and the transfer of heat from the melt to the coolant. The mixing process itself is described by giving the contact area as a function of time, i.e., by specifying $A_h(t)$. The increase in contact area during mixing can be assumed to be exponential.

$$A_h(t) = A_{ho} * e^{kt} \quad (17)$$

where A_{ho} is the prefragmentation contact area and k is a fragmentation parameter (which would be dependent on melt and coolant properties). The exponential form was chosen because that is the form that the area increase would take if the fragmentation process occurred by continuing division of droplets at a characteristic time interval. The heat transfer is treated as a 1-dimensional, unsteady-state conduction problem. This results in a thermal penetration distance, z , which is proportional to $(\alpha_H t)^{1/2}$, where α_H is the thermal diffusivity of the hot fluid.

$$z = k' * (\alpha_H t)^{1/2} \quad (18)$$

The product of the contact area, $A_h(t)$ and the thermal penetration distance, z , is the volume of the hot fluid that has interacted thermally with the coolant. The ratio of that volume at time t_1 to the total volume of the hot fluid can be equated to the mixing factor.

$$f_{mix} = \frac{A_h(t_i) * z(t_i)}{M_h/\rho_h} = \frac{\rho_h * A_{ho} * e^{k * t_i}}{M_h} * k' * (\alpha_H t_i)^{1/2} \quad (19)$$

We can define $\rho_h * A_{ho} / M_h = 1/d_{ho}$, where d_{ho} is a characteristic prefragmentation hot fluid dimension. Then,

$$f_{mix} = \frac{k'}{d_{ho}} * (\alpha_H t_i)^{1/2} * e^{k * t_i} \quad (20)$$

The values of k' from standard unsteady-state heat conduction theory is 4. This would be the correct value to use if all of the surface area was available throughout time interval t_i . However, new surface area is continually being created as fragmentation proceeds, so that thermal penetration is smaller for some of the area. It can be shown by solving a convolution integral that k' should lie between 1 and 1.5 for the expected range of area expansions.

The exponential term, e^{kt_i} , is the ratio of the final area to the initial area. For spheres, when the total volume is constant, the area ratio is given by

$$\frac{A}{A_{ho}} = \frac{N d^2}{N_{ho} d_{ho}^2} = \frac{d_{ho}}{d} \quad (21)$$

where N_{ho} = initial number of melt particles and N = final number of fragmented particles. Thus, kt_i can be interpreted as $\ln d_o/d$ where d is the diameter of the fragmented particles. For fragmentation ratios of 100 to 1000, $kt_i = 4.6$ to 6.9. Thus if t_i is on the order of 1 millisecc, $k \approx 5 \times 10^3 \text{ sec}^{-1}$.

It is possible to estimate the order of f_{mix} for the smelt water system. The thermal diffusivity of smelt is about $0.0018 \text{ cm}^2/\text{sec}$. t_i can be assumed to be 1 millisecc. The prefragmentation diameter can be taken to be about 2.5 cm (1 inch). Then

$$f_{\text{mix}} = \frac{1.5}{2.5} / \frac{0.0018 \times 0.001}{e^{5 \times 10^3} \times 0.001} = 0.12$$

Thus, it is not unreasonable to expect the mixing efficiency to be on the order of 10% for the smelt-water system. Similar, or slightly higher values might be expected for other systems such as thermite and water.

It appears reasonable to assume that f_{mix} is determined by the properties of the two fluids, the initial state of intermixing, and possibly the magnitude of the triggering impulse, and is not dependent on any global dimensions of the system.

The coherency factor can be looked on as a ratio between the volume of the system able to participate in a coordinated interaction and the total volume of the system. It would be expected to be dependent on the size of the system. For the spatially homogeneous case, the system size can be characterized by a single parameter, L_g , defined by $L_g = [M_h/\rho_h + M_c/\rho_c]^{1/3}$. This can be considered to be a global characteristic length for the system. It is not unreasonable to assume that the coherency factor would be a function of L_1/L_g , where L_1 is the characteristic interaction length discussed earlier. It is clear that $f_{\text{coh}} \rightarrow 1$ as L_1 becomes $> L_g$, and that f_{coh} will become small as L_1 becomes $\ll L_g$. The exact form of the dependence will depend on the "dimensionality" of the explosion. If the disturbance is propagating as a one-dimensional wave, we could expect a linear dependence of f_{coh} on L_1/L_g . If the disturbance is propagating three-dimensionally, we could expect f_{coh} to depend on $(L_1/L_g)^3$. In general one can use a power law relation,

$$f_{\text{coh}} = k''(L_1/L_g)^n \quad (22)$$

where n is a power between 1 and 3. The "dimensionality" which determines n will be dependent on the constraints existing in the system, and could be very difficult to predict. The coherency factor used here defines the interactive region around a single triggering point. In actual cases, such as the smelt-water explosions, multiple explosions may occur and a violent interaction in one region may trigger one someplace else. In these cases, the energy releases from each interaction would be added.

It is only possible to make rough estimates of f_{coh} . The intermediate scale experiments with thermite-water, discussed earlier, gave $F \approx f_h = 0.01$ to 0.1. Since f_{mix} could be expected to be about 0.1, f_{coh} ranged from 0.1 to 1.0. The global dimension of these systems, L_g , was apparently on the order of 1 ft. Interaction lengths are difficult to estimate. Propagation velocities of 200 to 600 m/sec were reported for thermite-water. If the interaction time is 1 millisecond, interaction lengths would range from about 0.5 to 1.5 ft. This appears reasonable. Since confinement (which would tend to lower n) tended to give somewhat higher efficiencies, n must normally be > 1 . The data would not be incompatible with a situation where $k'' \approx 1$, $n \approx 2$, and L_1/L_g ranged from 0.5 to 1.5. Note f_{coh} cannot be greater than one, so if $k'' (L_1/L_g)^n > 1$, $f_{coh} = 1$.

For systems, such as the recovery boiler, where the system dimensions are not homogeneous, we need to introduce another characteristic dimension, l_{min} , which is the minimum system dimension. For example, in the recovery furnace, $l_{min} = \text{depth of the smelt + water layer}$. In this case, the efficiency needs to be reduced by another factor, (l_{min}/L_g) , the ratio of the minimum characteristic length to the global characteristic length.

Thus the scaling criteria for the intermediate region can be summarized by

$$F \approx f_h = k'' \left(\frac{L_1}{L_g}\right)^n \left(\frac{l_{min}}{L_g}\right) f_{mix} \quad (23)$$

where f_{mix} depends on properties, the initial state of subdivision and trigger pulse magnitude, but not system size. The parameter k'' will be on the order of 1 and $n \approx 2$. L_1 would depend on properties of the two fluids, but would be expected to be on the order of one foot in magnitude.

Conclusions

Energy conversion efficiencies in steam explosions are normally a small fraction (< 10%) of the thermodynamic energy conversion efficiencies. The only exception is when small amounts of coolant are effectively dispersed in a large amount of melt. This latter case has minimal industrial importance because the magnitude of the energy release is small, since it is limited by the amounts of coolant.

Smelt-water explosions in recovery furnaces have energy conversion efficiencies generally in the range of 0.1 to 1% of the thermodynamic efficiencies. This is about one order of magnitude lower than efficiencies obtained with intermediate scale thermite-water experiments. Part of this difference may be due to the higher thermal diffusivity for thermite, but it is mainly due to the geometry of the smelt-water system in a recovery boiler. Smelt (and water) are present as wide, shallow pools, and the explosions are localized and do not involve the global smelt-water system. When calculated on a localized basis, the smelt-water efficiencies are about the same fraction of the thermodynamic efficiency as are those for thermite and water.

A simplified engineering analysis of steam explosions was developed which allows thermodynamic calculations to be used to estimate explosion energetics and which provides means for estimating the effects of system size. According to this analysis, the fraction of the thermodynamic efficiency which is actually realized depends on three multiplicative factors: a property dependent factor, a factor dependent on the global characteristic dimension, and a factor related to inhomogeneities in system dimensions. In general, the analysis suggests that energy conversion efficiencies decrease as the size of the system increases, particularly as system dimensions exceed an "interaction length" which appears to be on the order of one foot. The analysis does provide a plausible interpretation of the experimental results.

References

1. Energetics of smelt-water explosions, NUREG/CR-4745.
2. Hicks, E. P.; Menzies, D. C. Theoretical studies of the fast reactor maximum accident, ANL-7120, Oct., 1965:654-70.
3. Keenan, J.; Keyes, F. Thermodynamic properties of steam, John Wiley & Sons, New York.
4. Anderson, R. P.; Bova, L. Final report on the small scale vapor explosion experiments using a molten NaCl-H₂O system, Argonne National Laboratory, ANL-76-57, April, 1976.
5. Anderson, R. P.; Armstrong, D. R. Comparison between vapor explosion models and recent experimental results, AIChE Symp. Series 138(70):31(1973).
6. Bergman, S.; Laufke, H. Recovery boiler explosions, The Swedish Steam User Association SPCI Report No. 35 (1978).
7. Buxton, L. D.; Benedick, W. B. Steam explosion efficiency studies, SAND 79-1399 (NUREG/CR-0947), Sandia Lab., NM (1979).
8. Mitchell, D.; Evans, N. Effect of water to fuel mass ratio and geometry on the behavior of molten core-coolant interaction at intermediate scale. Proc. of the Intl. Meeting on Thermal Nuclear Reactor Safety, Chicago, IL, 2:1011(1982).

Table 1. Energy conversion efficiencies for smelt-water explosions.

Incident	Deformation Energy, Btu	Amount of Smelt, lb	Smelt Temp., °F	Amount of Water, lb	Water Temp., °F	Actual Efficiency, %	Thermodynamic Efficiency, %	Ratio of Actual to Thermo. Eff., %
1	41,500	88,000	1450	2,000	212	0.113	2.3	4.9
3	5,500	10,000	1400	20,000	212	0.130	16.6	0.78
6	5,200	23,800	1450	8,000	212	0.050	20.5	0.24
8	1,740	8,100	1600	> 16,000	212	0.045	< 17.5	> 0.26
10	28,000	55,700	1600	2,000	212	0.106	3.5	3.0
12	3,100	33,000	1400	10,000	212	0.034	20	0.12
13	150	6,000	1600	1,000	212	0.005	14	0.04
19	8,900	25,200	1600	> 16,000	212	0.074	< 22.5	> 0.33
25	1,800	28,000	1700	6,000	110	0.013	15.5	0.08
27	14,000	43,000	1400	4,000	160	0.078	9.1	0.86
34	225	9,300	1500	2,000	80	0.005	15	0.03
36	9,200	30,000	1600	> 16,000	212	0.064	< 22.5	> 0.28
37	6,600	16,500	1600	> 16,000	212	0.084	< 21.5	> 0.39
39	1,360	21,600	1500	> 16,000	212	0.014	< 22	> 0.06
42	11,800	7,800	1400	> 16,000	212	0.37	< 15.6	> 2.4
43	14,000	25,200	1500	10,000	160	0.125	20	0.63
45	4,500	33,000	1500	8,800	212	0.031	19	0.16
48	5,300	24,000	1450	6,000	212	0.051	19	0.27
Diss. tank	1,000	7,500	1700	162,000	100	0.023	0	---

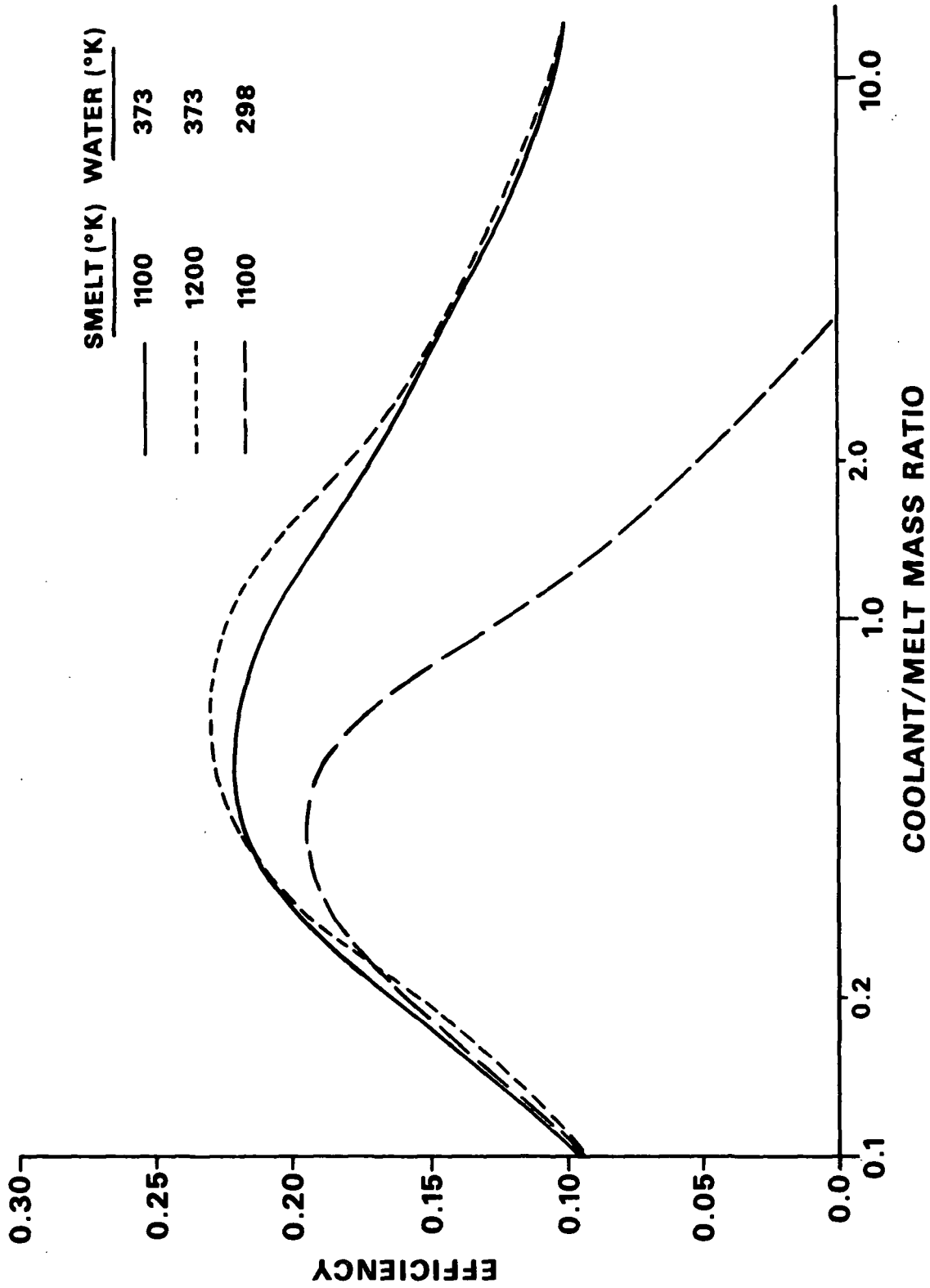


Figure 1. Thermodynamic energy conversion efficiencies for the smelt-water system.

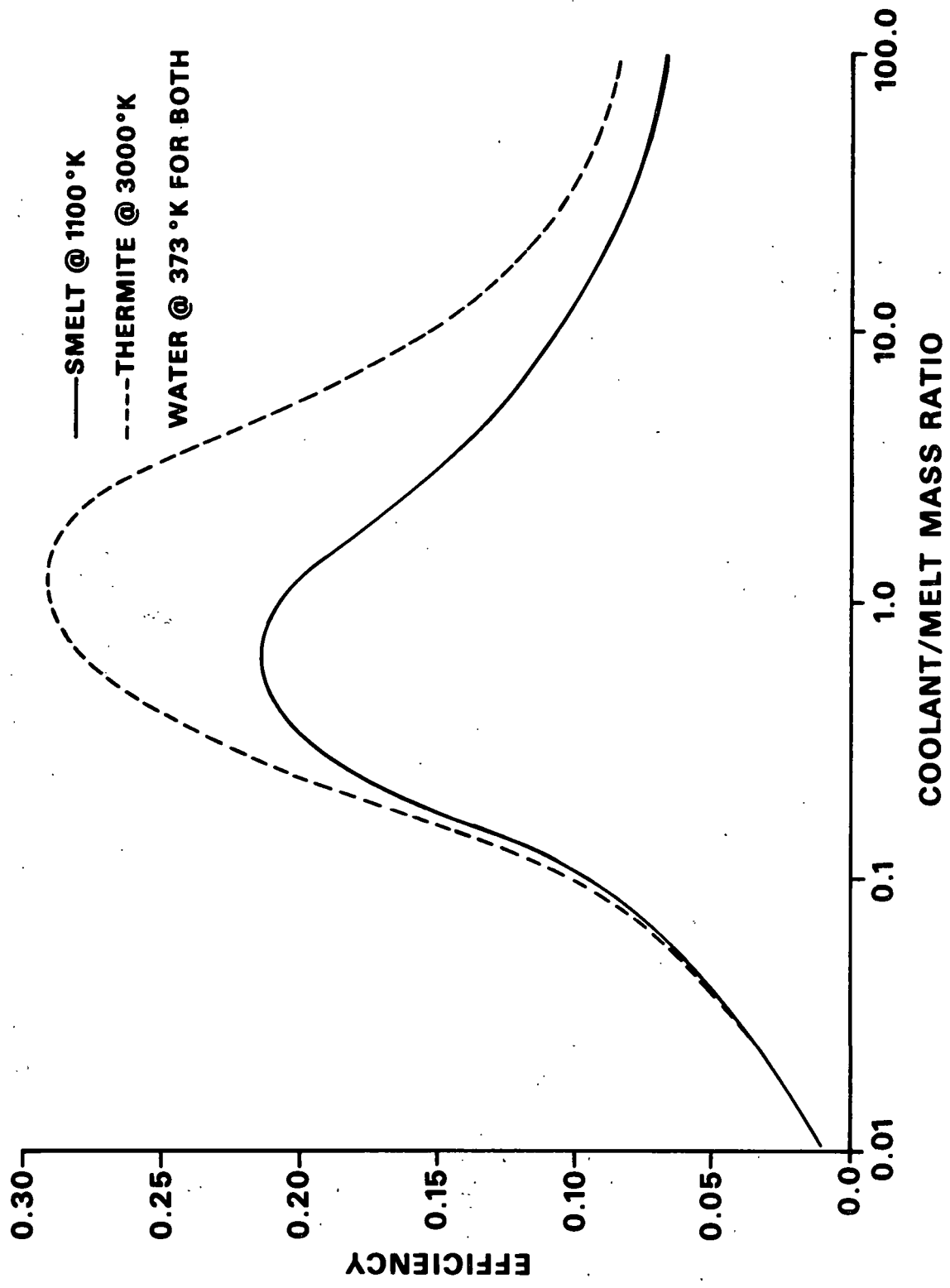


Figure 2. Comparison of thermodynamic efficiencies for smelt-water and thermite-water.