

1978 Award Lecture

THE DYNAMICS OF RUNAWAY SYSTEMS

The 1978 ASEE ChE Division Lecturer was Dr. Theodore Vermeulen of the University of California, Berkeley. The 3M Company supports this annual award.

Dr. Vermeulen, born in Los Angeles, completed his B.S. and M.S. in ChE at CalTech, and his Ph.D. in physical chemistry at UCLA. He did catalytic research for Union Oil for two years and later worked six years in process development and research planning for Shell Development. He then joined the University of California, Berkeley, serving as founding chairman for ChE from 1947 to 1953, and being advanced to professor (his present post) in 1951. He has been a Fulbright Professor and a Guggenheim Fellow, and received AIChE's William H. Walker Award in 1971.

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SCIENTIFIC ANALYSIS OF explosions and flames is not viewed today as an area of interest or concern for us as chemical engineers. Nevertheless we often bear the responsibility for assuring that no harm will come through explosion or flame to a chemical plant or refinery we are operating or planning, or to a laboratory experiment we are conducting. Combustion takes on new importance as we strive for higher energy efficiency, avoidance of pollution, and use of alternate fuels. Intellectually, the "runaway" phenomena can enrich our perceptions of thermodynamics, kinetics, and thermal and mass transport. The award from ASEE of this Lectureship, which has been established through the generosity of the 3M Company, has enabled me to focus my attention on

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"runaway" systems and to share my findings with you about aspects of these areas which appear accessible, interesting, and valuable.

The area of process dynamics comes close to dealing with runaway problems, but even there the emphasis is more on preventing the runaway than on analyzing it.

THE ANATOMY OF AN EXPLOSION

NUCLEAR EXPLOSIONS ARE the most researched, most dramatic, and most unwanted. Scale-down, rather than scale-up, will relate this prototype to conventional applications. The mushroom cloud (Figure 1) is not unique to nuclear explosions; it occurs also even in middle-sized explosions on land or in fairly small "shots" under water. Every explosion has both a build-up and a let-down stage, and the mushroom cloud is part of the let-down. Samuel Glasstone's book "The Effects of Nuclear Weapons" is the source of Figure 1 and of the following description of a nuclear "blast":

The time scale for a nuclear explosion is so short that we sense only the overall result. At the instant the critical mass for nuclear fusion is brought together, only a few neutrons are present. Fission begins promptly, with a reaction time of about 10^{-8} seconds (10 nanoseconds). Each fission step consumes one neutron and produces two neutrons or a fraction more. A kiloton (as TNT) of energy release requires production of 10^{23} neutrons, or about 53 generations of reaction time—530 nanoseconds. A megaton requires 1000 times more—another 7 generations, that is, another 70 nanoseconds. Thus the build-up lasts less than one microsecond, and the bulk of the

“detonation” occurs in less than one-tenth of a micro-second.

The energy released raises the local temperature to more than 10 million degrees Kelvin, and the local pressure to more than 1 million atmospheres. X-rays rapidly radiate into the surrounding atmosphere, heating the air so high that it too becomes luminous. The mixture of air and weapon residue forms a fireball which grows outward and upward 500 feet in the first millisecond. This volumetric rate of growth persists, so that the fireball spreads to more than a mile across within 10 seconds. At this time its center of mass is rising about 400 ft/sec. The light intensity per unit exposed area of fire ball is greatest at 1 millisecond, but the total light emitted from the fireball peaks at 10 seconds. The expansion and upward motion continue much longer. In about 1 minute, the fireball is 4 miles above the burst point; it no longer emits visible light; and it has become a toroid, or “mushroom cloud.” An updraft of drawn-in air follows the cloud. A thermonuclear bomb will give a larger cloud than one only involving fission, but the pattern of behavior does not change.

The blast wave reaches its peak velocity (about 5 miles/sec) and peak pressure at the end of the build-up. It pulls ahead of the spent charge, and travels outward at sonic velocity—that is, at over 1000 ft/sec—with one to two atmospheres of maximum overpressure, which persist for one second or longer at each point. Its intensity is heightened by reflection of the shock wave from the ground, and by the kinetic energy of the 500 ft/sec wind accompanying the wave. In another second or so, a suction wave arrives with an underpressure of up to one-fourth of an atmosphere, and this causes additional damage. The blast or shock wave subsides with increasing distance from the source, but an overpressure of one fifth of an atmosphere may be felt 2 miles away from a small nuclear explosion and 10 miles away for a large one.

To summarize the energy balance, one-third of the energy leaves as radiation over all wavelengths; one-third is dissipated as purely thermal molecular energy; and one-

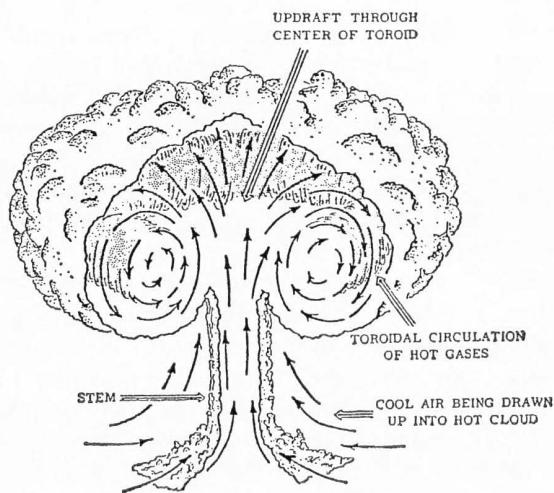


FIGURE 1. Toroidal circulation inside the radioactive cloud from a nuclear explosion (after Glasstone)

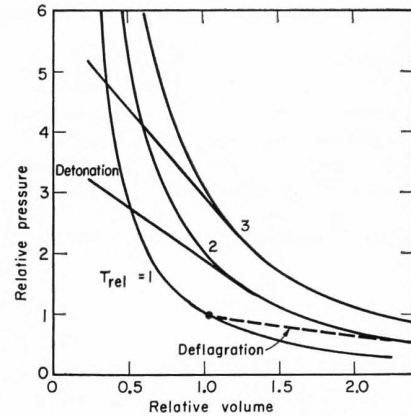


FIGURE 2. Hugoniot curves for shock waves under let-down and build-up conditions

third is discharged by the blast wave as pressure energy, attenuated by friction and turbulence. On a still larger scale of nuclear explosions, novas are believed to be exploding planets; and supernovas, exploding stars.

As we adapt to these concepts, we become interested first in how to identify potential runaway; then in how to monitor and control potential runaway, to reduce its chance of happening; and finally to strive for the supermonitoring and supercontrol that might interrupt a runaway already started. For a nuclear bomb, we would have to detect the neutron build-up within 30 nano-seconds, and take evasive action within 300 nano-seconds, in order to blunt the harmful effects of the bomb. If this disruption were done by a laser blast, the laser would have to be located within 50 meters' distance from the bomb.

THE RANKINE-HUGONIOT DIAGRAM

PRESSURE AND VOLUME ARE familiar coordinates to us, along with their typical constant-temperature and constant-entropy paths; but the curves applicable to shock waves at sonic velocity, shown in Figure 2, involve generally unfamiliar balances.

The curved paths in the figure represent the passage of a one-dimensional compression wave through an ideal gas. The Bernoulli relation or equation of motion relates the velocity change to the pressure change, and the energy balance records the temporary conversion of kinetic energy to internal energy. With $\pi = p/p_0$, $\phi = v/v_0$, and $\theta = T/T_0$, the temperature and pressure ratios follow the relation:

$$\theta = \frac{2\gamma + 1 + \pi}{2\gamma + 1 + (1/\pi)}$$

If frictional dissipation and spherical geometry are neglected, for a shock wave travelling through air after the build-up stage, the Rankine-Hugoniot curve shows the compressed condition of the gas corresponding to the pressure rise in the shock.

with, for example, $\gamma = c_p/c_v = 1.4$ for air. In the event π is very large, the least value of the volume ratio $\phi (= \theta/\pi)$ is $1/(2\gamma+1)$, or 0.26 for air. Hence every different starting point will have its particular Rankine-Hugoniot curve. Also, the slope is steeper than for isentropic compression at any given ϕ . It is worthwhile to note that the Rankine-Hugoniot condition is not a differential equation; rather, it is a finite difference relation, implying a mathematical discontinuity between start and finish.

If frictional dissipation and spherical geometry are both neglected, for a shock wave travelling through air after the build-up stage, the Rankine-Hugoniot curve shows the compressed condition of the gas corresponding to the pressure rise in the shock. Under ideal conditions, the gas will revert to its initial condition when the shock has passed, since the original balances again apply, and a reciprocal π gives reciprocal θ and reciprocal ϕ .

We consider next the behavior of the shock during the build-up period. When combustion occurs, the gas at a given point does not revert to its starting condition, but instead its return to initial pressure is characterized by higher volume and temperature. This expansion reinforces the shock, causing it to increase steadily in pressure. The temperature reached by the combusted gas at base pressure is represented by a Raleigh line, and by the Hugoniot curve to which the Raleigh line becomes tangent. At an early stage of build-up, for example, π reaches 2.7, and a Raleigh line carries the mixture to Hugoniot curve 2; later π reaches 4.7, and another Raleigh line carries the mixture to curve 3.

As combustion occurs in the high-pressure zone of the shock, the thermal-energy release tends to shift the gas from a lower to a higher isotherm. Traveling at the relevant sonic velocity, the shock traverses equal masses of gas in equal time (corresponding to a constant mass velocity of gas through the shock). The resulting tendency toward higher momentum must be offset by a drop in pressure, which accounts for the linear be-

havior of the combustion path (the Rayleigh line). Thus,

$$p + \left(\frac{u_0}{v_0}\right)^2 v = \text{constant}$$

where u_0 is the sonic velocity at the point of maximum compression.

The reader will note that Figure 2 is drawn on linear scales for the sake of simplicity. The wide range of pressures and temperatures ordinarily encountered in an explosion would generally justify the use of logarithmic coordinates for such plots.

CRITICALITY

A SMOOTHLY RUNNING nuclear reactor, or a steady-state star like our sun, has crossed one kind of threshold. It appears that there must be one barrier—one criticality condition—for burning nuclear fuel; and another, higher, degree of criticality for setting off a nuclear explosion.

Sometimes the burning condition is not a stable state, but an antistable one, only kept in balance by oscillatory controls—a push to increase the rate, a pullback to reduce the rate. In this case the measure of dynamic stability lies in the adequacy of the combination of controls with the reacting material, and not merely in the properties of reacting material considered by itself. If fluctuations in the system cause an overriding of the controls, they may quench the burning on one hand, or they may launch an explosion on the other.

An analogous situation exists with chemical explosions and chemical flames. A flame is not usually self-igniting. Within a certain range of concentrations bounded by "critical" values, the reaction mixture when ignited will produce a flame that is self-sustaining. Inside a narrower range of concentrations, bounded again by "critical" values, the flames will reach sonic velocity and thereby will attain the condition of detonation.

Neutron reactions are by nature "chain" reactions, and any branching chain which allows the number of neutrons to increase without limit is by nature "explosive". So too are there chemical reactions of branching-chain type, involving molecular fragments and single atoms, all collectively termed free radicals. If the chain branching is moderated, so that the concentration of radicals tends toward a steady-state value, we might ex-

Continued on page 205.

AWARD LECTURE

Continued from page 158

pect to avoid explosion. However, often another consideration arises.

Temperature rise has an accelerative effect on chemical reaction rate, which is without direct parallel in nuclear reactions. In addition to chain runaway, we may encounter thermal runaway of any strongly exothermic reaction, limited only by its respective adiabatic-maximum temperature rise. Again the velocity at which the reaction spreads determines whether smooth burning ("deflagration") or explosion ("detonation") results.

It is a question of whether the rate increases because the temperature rises, or whether the temperature rises because the rate increases. The thermal system is controlled by removing heat, while the chain reaction is controlled by removing neutrons or (in the chemical case) free radicals. In one case, we select a container lining for its thermal conductivity; in the other, for its capacity to absorb or adsorb the chain carriers.

CHEMICAL REACTION LIMITS

Combustion, thermal pyrolysis, and organic photochemistry all occur by multi-step reactions involving the production and consumption of free radicals. Most studied of the combustion reactions as a prototype, and still imperfectly understood, is the hydrogen-oxygen reaction—cited in almost all physical chemistry texts, and explained adequately and correctly in almost none.

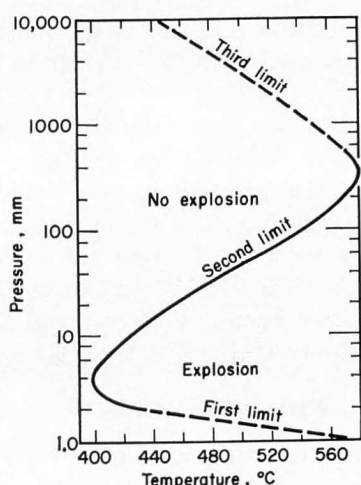


FIGURE 3. Ignition limits for stoichiometric hydrogen-oxygen mixture in a 15-cm spherical vessel (after Lewis and Von Elbe)

Figure 3 is a classic diagram of the ignition limits for H_2 with O_2 , developed largely through the pioneering work of Bernard Lewis and Guenther Von Elbe in the U.S. Bureau of Mines during the 1940's. This diagram applies to stoichiometric properties of hydrogen and oxygen, which give a flame speed that usually exceeds sonic velocity; thus the ignition limits are also explosion limits. If we start at very low pressure, at a given constant temperature (say, $450^\circ C$), and move upward in pressure, we

- start in a zone of slow, measurable reaction
- advance through the "first explosion limit" into a region of high temperature and fast reaction.

If we start at a still higher pressure (say 1 atm.), and then lower the pressure, we

- start in a zone of slow, measurable reaction
- drop through the "second explosion limit" into the same high-temperature fast-reaction region we had previously encountered.

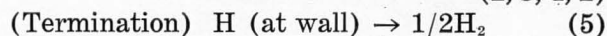
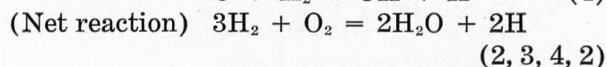
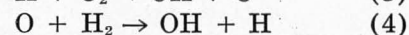
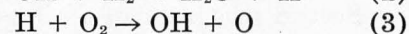
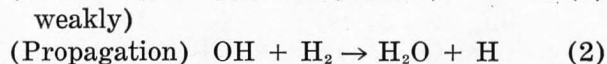
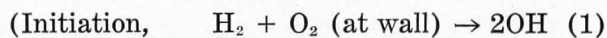
Starting again at 1 atm. and increasing the pres-

It is a question of whether the rate increases because the temperature rises, or whether the temperature rises because the rate increases.

sure, we

- advance through the "third explosion limit" into a new overlying region of high temperature and fast reaction.

First Explosion Limit. If we describe accurately the chemical behavior which occurs in the measurable region, we find that the kinetics will predict the existence and nature of the explosion limits. For steady-state concentration of radicals, the rates of all the propagation steps must be equal, and also, below the first explosion limit, collision of radicals with the vessel walls must occur at an equivalent rate:



At steady state, then, the net production of radicals is

$$k_1(H_2)(O_2) + k_3(H)(O_2) - 2[K_5/(Pr^2)](H) = 0.$$

where the parenthesis denote gas-phase concen-

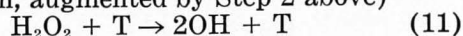
trations for partial pressures, (if the coefficients are adjusted appropriately), and K_5/P is an effective diffusivity for H atoms based on an assumed uniform concentration through the entire sphere of radius r , at total pressure P . If we solve for (H) from this relation, then take the total rate equal to that of step 3 and substitute (H) into that rate under constant-volume conditions, the total steady-state reaction rate is given by:

$$-\frac{d(O_2)}{dt} = \frac{k_1 k_3 (H_2) (O_2)^2 P}{2[K_5/r^2] - k_3 (O_2) P}$$

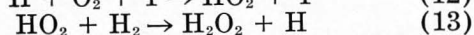
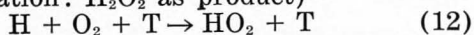
Because (O_2) is proportional to P , an increase in P will bring on explosion by causing the denominator to approach zero, and the quotient to approach infinity.

Second Explosion Limit. In the explosive region between the first and second limits, reaction steps 2, 3, and 4 continue to predominate. As the total pressure increases, a three-body reaction competing with step 3 (with T the "third body") grows in and forms the radical HO_2 and its daughter product hydrogen peroxide. Above the second limit the initiation and termination steps have shifted from the vessel surface to the near-homogeneous phase within. After a short induction period, the reaction path in the steady-state region above the second limit can be represented as follows:

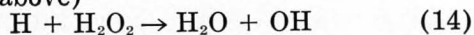
(Initiation, augmented by Step 2 above)



(Propagation: H_2O_2 as product)



(Propagation: H_2O as product, by addition of Step 2 above)



(Termination)



We now identify a steady-state reaction condition involving three independent relations.

First, the rate of oxygen consumption (excluding step 3) is

$$k_{12}(H)(O_2)P = k_{13}(HO_2)(H_2)$$

Second, the rate of H_2O production is

$$k_2(OH)(H_2) = k_{14}(H)(H_2O_2)$$

Third, the net production of radicals is

$$k_{11}(H_2O_2)P + k_3(H)(O_2) - k_{15}(H)(HO_2)P = 0$$

Excluding step 3, we have

$$(HO_2) = \frac{k_{11}k_{12}P}{k_{13}k_{15}} \left[\frac{(H_2O_2)(O_2)}{(H)} \right]^{1/2} \\ \cong K (H_2O_2)^{1/2} P^{1/2}$$

This relation indicates that the H_2O_2 concentration is controlled by the termination reaction.

It will grow rapidly, ahead of the steps producing H_2O_2 , until a limiting ratio to the reactants is reached (which increases with total pressure), and will then subside slowly as the reactants are consumed. At high H_2O_2 a different termination step may predominate ($2HO_2 \rightarrow H_2O_2 + O_2$), but this will produce very little change in the kinetic relations.

Finally, the total rate (including step 3) is approximately

$$-\frac{d(O_2)}{dt} = \frac{(k_{11}P + k_3)k_{11}(H_2O_2)(O_2)P}{k_{15}K(H_2O_2)^{1/2}P^{3/2} - k_3(O_2)} \\ \approx \left[\frac{k_{11}k_{12}k_{13}}{k_{15}} \right]^{1/2} (H_2O_2)^{1/2} (O_2) P^{-1/2}$$

As P falls, the denominator tends toward zero, giving a runaway rate. The second explosion limit (unlike the first and the third) is seen to be relatively independent of the vessel radius.

Third Explosion Limit. Considerable ingenuity has been expended by researchers in the field in formulating chain-branching reactions that would explain the uppermost explosion limit. However, the rates measured in this region do not give any indication of impending chemical runaway, such as is seen near limits 1 and 2. If we use the existing rate data or rate equations to predict where normal runaway should occur in a spherical vessel of 3-inch radius, by a calculation method to be described below, the prediction places it almost exactly at the experimental locus of the third explosion limit. If instead we assume that some type of chain branching occurred in this region which accelerated the kinetics, we then predict that a thermal runaway would occur at a lower temperature or pressure than the experimental value.

The mechanism given above has been simplified, and other radicals are also present; but it appears that the proponents of a chemical runaway are neglecting the temperature difference that develops between the reaction vessel contents and the isothermal outside wall of the vessel. The problem has not been laid to rest, but the case for a thermal runaway here is very strong.

THE THERMAL RUNAWAY LIMIT

THE PRESUMED THERMAL ignition limit for a hydrogen-oxygen mixture is one of a myriad of cases of "spontaneous" ignition. Runaway occurs if the body of combustible mixture that is heated is large enough so that the heat released

cannot all be lost by conduction and convection, allowing the temperature (and reaction rate) to rise to a point where the mixture can react to completion. If this reacted portion is part of a larger body of combustible mixture, the heat liberated in this way is usually sufficient for combustion to spread through the entire mixture. Every time you strike a match, or a spark plug fires in your automobile engine, the same principle is involved.

We will now examine the criticality condition for a spherical vessel which is kept isothermal at the vessel surface. For a given mixture composition, the criticality can be expressed in terms of a mass or volume for a given temperature, or a surface temperature for a given mass or a given dimension (thus the concept of ignition temperature, which may not be truly constant), or even as a value for the rate coefficient at the vessel surface.

Let R be any radius, R_s the entire radius of the vessel, and r the relative radius R/R_s . Let k_s be the "rate of conversion" (fractional conversion per unit time), or first-order rate constant, for unreacted mixture at the surface temperature. The effect of temperature on rate is approximated by a linear exponential term: $k = k_s \cdot \exp(\Psi\theta)$. Here θ is the fractional temperature rise, with $\theta = 1$ at the adiabatic maximum temperature and $\theta = 0$ at the vessel surface; θ increases from 0 at the surface to θ_c at the center of the sphere. The coefficient Ψ is related to effective activation energy E by the relation $\Psi = EJ/RT_s^2$, where J is the adiabatic maximum temperature rise. Also, k_H is the effective thermal conductivity of the reaction mixture, and Λ is the heat release per unit volume of reaction mixture for complete conversion.

Following Frank-Kamenetskii and Damköhler, we may now equate the integral for heat release over the entire vessel to the heat-transfer rate

from the mixture to the vessel wall:

$$\Lambda \cdot \frac{4}{3} \pi R^3 k_s \int_0^1 e^{\Psi\theta} r^2 dr = 4\pi R k_H J \left(\frac{d\theta}{dr} \right)_s$$

With the aid of the spherical heat-conduction equation (much as in the derivation for effectiveness factor of spherical catalyst particles) we can establish the entire profile of θ vs. r , and substitute the result into our present equation.

The temperature gradient $d\theta/dr$ at the surface increases steadily with θ_c . We find that no steady state exists if $\Psi\theta_c$ is greater than 1.6, or $\exp(\Psi\theta_c)$ greater than 5. The corresponding value of the dimensionless group formed from the variables in the equation is

$$[k_s \Lambda R^2 / k_H J \theta_c] = 2.1$$

An alternative group can be formed by introducing $\Psi\theta_c$:

$$[k_s \Lambda R^2 \Psi / k_H J] = 3.3$$

All these values are upper limits for avoiding ignition, and lower limits for achieving ignition.

It should be noted that the subgroup $k_H J/\Lambda$ is the same as thermal diffusivity. Hence either of the above groups can be viewed as the thermal counterpart of the Thiele modulus for spherical catalyst particles, which is used to calculate the effect of mass diffusivity on the effectiveness factor.

For a well-stirred spherical tank reactor, with the entire contents at a single concentration and a single temperature, similar criteria again apply; the batch and continuous-flow cases are not very different. For this reactor, K^2/k_H is replaced by R to the first power divided by U , the overall heat-transfer coefficient. Again the mathematical analytic solution ceases to exist when the critical value is reached, the latter group above now being e or 2.718 instead of 3.3.

TABLE 1
Flammability Limits In Air

COMPOUND	MOLE-FRACTION OF COMPOUND				TEMPERATURE, °R.	
	LOWER	STOIC	MAX. VEL.	UPPER	MAX. VEL.	IGNITION
Hydrogen	.040	.258		.745		1500
Methane	.050	.095		.150		1535
Ethane	.033	.056	.063	.125	4040	1340
Acetone	.030	.050	.058	.116	3820	1500
n-Butane	.017	.031	.035	.103	4060	1270
n-Heptane	.010	.019	.023	.084	3980	940
iso-Octane	.008	.017	.019	.059	4020	1300

It is quite revealing to develop the temperature profile in the spherical reactor as an evolutionary problem on a programmable hand calculator. A value for the critical factor just 0.01% low results in a temperature 1.5% below the critical value. A value 0.01% too high leads to a very leisurely runaway. This close to the critical, an enormous time is required to creep past the critical region. This brings to mind the ignition and eventual devastating detonation of kilotons of ammonium nitrate in Texas City, Texas, on April 16, 1947.

With a plug-flow reactor cooled from outside, the sharp distinction between stability and instability disappears, and is replaced by the concept of *parametric stability*. A relatively steep transition occurs from a low conversion to a very high one within a narrow range of values of a dimensionless factor equivalent to the two groups given above. If any particular criterion of temperature or conversion is applied, say a temperature rise not more than x degrees, then a specific value of the factor can be applied as the control.

The rate of fractional conversion, referred to above, is a strong function of temperature and comparatively a weaker function of mixture composition. For any given type of fuel, the temperatures corresponding to the k_s values which fit the criticality criteria will always lie in a narrow range which can be defined loosely as "ignition temperature." Table 1 gives flammability limits for several combustible compounds, along with ignition temperatures measured for the stoichiometric mixtures. In every case, the lower and upper flammability limits are the mixtures having adiabatic maximum reaction temperatures which just reach the reference ignition temperature. This means that the flammability limits can be estimated quite accurately from a single value of ignition temperature. Also, one flammability limit can be calculated if the other has been measured.

The lower flammability limit always shows an excess of air over combustible which is greater than the excess of combustible over air for the upper flammability limit. The reason for the asymmetry is that CO_2 , the main product from lean-mixture combustion, has a high exothermic heat of formation; and that formation of CO , the main product from a rich mixture, is considerably less exothermic.

Ignition temperatures have the philosophic drawback that they seriously oversimplify the kinetics, and thus tend to obscure the detailed be-

havior of combustion systems. Essentially the rate of burning is considered zero below the ignition temperature, and infinity above. Our concluding section provides another instance of the advantages of detailed modeling.

ONE-DIMENSION MODELING OF PREMIXED FLAMES

WE HAVE ALREADY SEEN that combustion generally proceeds by a sequence of free-radical reactions. For a premixed gas, the flame sustains itself by projecting free radicals and heat backward into the oncoming cold feed. A very simple physical model of a flame results if we assume that the Lewis number is unity; that is, that the thermal diffusivity and mass diffusivity are the same. With this assumption the fractional extent of stoichiometric reaction matches the fraction of adiabatic temperature rise; conversion and temperature collapse into a single variable.

This method enables two partial differential equations to coalesce into a single 2nd-order ordinary differential equation, which involves (1) dimensionless length (a form of Peclet number), (2) dimensionless temperature θ or conversion f , (3) the activation energy factor ψ , and (4) a dimensionless maximum-temperature rate parameter involving the first-order constant k_{∞} . The dimensionless length and dimensionless rate constant each contain both the effective diffusivity D and the flame velocity U_0 . Any one kinetics, starting temperature, and diffusivity will converge for only one particular value of the rate constant; that is, the numerical integration does not converge on 100% conversion unless the right

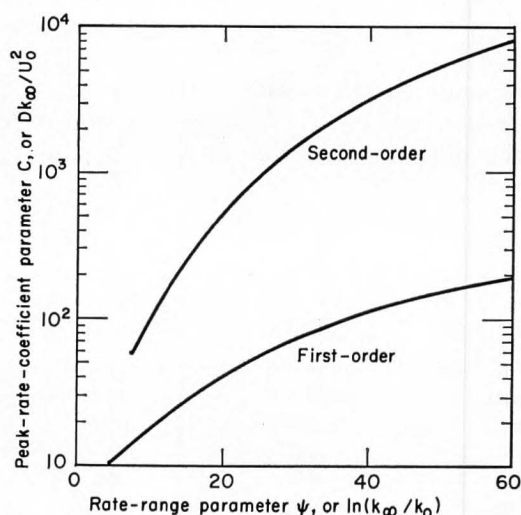


FIGURE 4. Effect of rate-range parameter on flame-velocity group

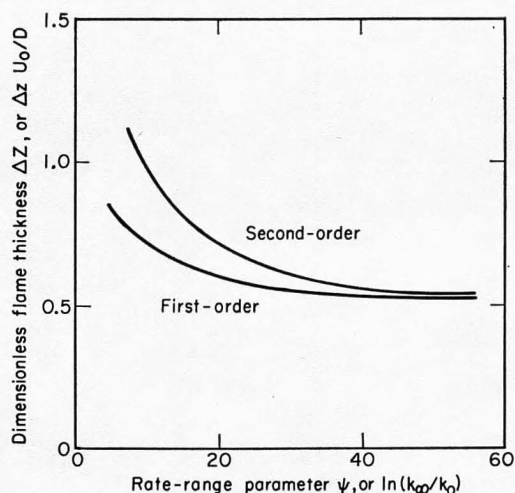


FIGURE 5. Effect of rate-range parameter on flame-thickness group

dimensionless rate constant is used which corresponds to the right U_0 .

We let X represent both the fraction converted f and the dimensionless temperature rise θ ; $Y = 1 - X$; D , both the mass diffusivity and the thermal diffusivity; z , distance within the flame, measured from a reference plane (e.g., where $X = 0.05$); Δz , the specific distance between $X = 0.05$ and $X = 0.95$; α , the order of reaction, assuming stoichiometric proportions of the reactants; $Z = zU_0/D$; and $C = Dk_{\infty}/U_0^2$.

The ordinary differential equation is

$$U_0 \frac{dX}{dz} + D \frac{d^2X}{dz^2} = k_{\infty} e^{\psi(1-X)} (1-X)^{\alpha}$$

In dimensionless form,

$$-\frac{dY}{dZ} - \frac{d^2Y}{dZ^2} = C e^{-\psi Y} Y^{\alpha}$$

The results of numerical integration of this equation, for $\alpha = 1$ and 2 , and for different ψ , are given in two new plots. Figure 4 gives C as a function of ψ , and can be used to determine the flame velocity U_0 from the rate coefficient k_{∞} , or vice versa; Figure 5 gives ΔZ , also as a function of ψ , and can be used with U_0 to define the true flame thickness. If one has an experimental flame thickness and does not know D , the figures are used in reverse order.

The ΔZ group has been called the Karlovitz number, after a longtime staff member of the U.S. Bureau of Mines. This group was observed empirically to be always in the vicinity of 1, lending credence to the approximations in our calculation.

The low- ψ , low- k_{∞} end of these curves once

more represents the point where the solution vanishes—i.e., the flammability limit, which may involve a flame speed of only a few feet per second. It is a matter of convenience to use k_{∞} , rather than the starting value k_0 , as the rate constant; Figure 4 would show many more orders of magnitude if C contained k_0 . The flame velocity increases rapidly with increasing ψ , and sonic velocity is likely to occur in the rate of 25 to 40 for ψ .

These few concepts with their accompanying mathematical models go a long way toward eliminating the mystery that seems to surround flames and explosions. Let's work together to examine how and where they might be given increased attention in the undergraduate curriculum. □

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ChE stirred pots

THE CREATION

And in the beginning there was "Control." And Control created τ . And Control saw that this was good, but that τ was lonely, so Control created τ a mate and Control saw that this also was good. τ 's mate was called $\tau s + 1$. But before long $\tau s + 1$ led τ down the path of sustained oscillation. Control saw this and He was troubled. He granted τ and $\tau s + 1$ a transfer function to the land of instability where through the wonders of "Control" $\tau s + 1$ begat Gain. And before long $\tau s + 1$ also begat Routh. One day while tending the process, Gain became quite angry with Routh and rattled his array but good. And then Gain fled to the caves of Frequency Response, emerging only at odd multiples of τ to wash his B.V.D.'s and read the weekly edition of the "Control Gazette."

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