

## *Stochastic Modelling and Computational Sciences*

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### CHEMICAL INFLUENCES ON THE PROPAGATION OF SOUND.

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#### ABSTRACT

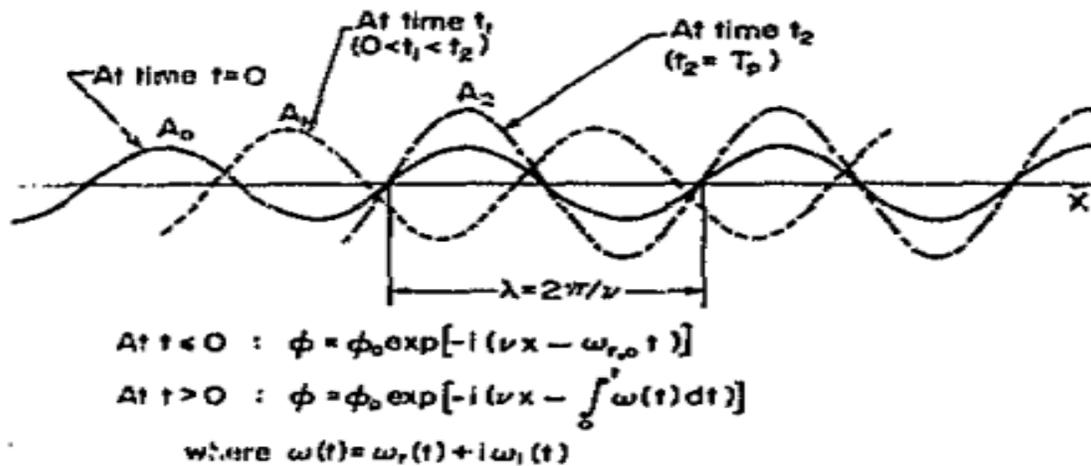
*A theoretical investigation of the relationship between sound propagation and chemical kinetics is showcased. An analysis of the equations for the propagation of a travelling acoustic wave in a chemically reacting, gaseous medium reveals that there are two main types of chemical effects: those resulting from acoustic waves that cause fluctuations in reaction rate and those resulting from chemical reactions that alter mean conditions. Many cases have been studied, and it is found that these coupled effects depend on activation energy, enthalpy of reaction, and ratio of chemical to acoustic time. They also have distinct qualitative features for exothermic and endothermic reactions. When exothermically time is long and composed with acoustic time, the primary effects are caused by fluctuations in the reaction rate. Acoustic waves are intensified in the case of exothermic reactions and diminished in the case of endothermic reactions when reaction rates rise with temperature. Within the validity range of this quasisteady analysis, the sound propagation speed is only marginally deducted from its isentropic frozen value. Changing the mean conditions is what causes the chemical effects when the reaction rate is constant. Here, the acoustic waves are amplified for endothermic reactions and attenuated for exothermic reactions, which is opposite to what is predicted for the quasisteady case. Additionally, effects on propagation speeds become more noticeable. The final results are highly dependent on activation energy when taking into account both types of chemical impacts. The qualitative effects are comparable to those noted for constant reaction rate in the situation of small activation energy, when the temperature has a negligible influence on the reaction rate.*

*Keywords: sound propagation, chemical kinetics, Acoustic waves, chemical effects,*

#### INTRODUCTION

In the study of problems involving instability in chemically reacting media of One fundamental important question in the study of instability in chemically reacting media (combustion instability, detonation wave structure, turbulence spectra in reacting flows, etc.) is what potential chemical effects might have on the creation, amplification, and propagation of acoustic waves.[1,2] indicates that if there is a suitable phase connection between the oscillating energy source and the acoustic density, then such effects are indeed conceivable. Rosen [3], for example, provided criteria for wave amplification when liquid droplets gasify when chemical action is considered a mass source. Research [4–7] on the relationship between flames and pressure waves also suggest a potential amplification. Research on the propagation of sound in an in viscid, no thermally conducting, until now dissociating gas [8, 9] demonstrates further that acoustic frequencies influence dispersion and absorption relations. Only the attenuation of pressure waves, nevertheless, have been documented. Such attenuation effects might arise from the presumption that, in its undisturbed state, the gas is at chemical equilibrium. It is envisaged that pressure waves can be amplified and that the pertinent amplification relations are frequency dependent when irreversible chemical reactions—including the temperature dependence of their rates—are taken into account. In fact, Nikolayev [10] predicted this outcome. It, however, only holds true for slow reaction speeds in relation to acoustic frequency.

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A right-traveling acoustic wave of fixed wavelength but varying amplitude and propagation speed in an infinite reacting medium.

This work examines in details those non equilibrium effects and presents theoretical results, showing coupling between chemical kinetics and sound propagation, for different activation energies and ratio of chemical to acoustic time and for both exothermic and endothermic reaction. Analyse the propagation of traveling-wave acoustic waves in an infinite-length, inviscid, nonconducting, stationary, chemically reactive gaseous medium. The placements of these waves are displayed in Figure I at three different times, where,  $T_p$  is equivalent to one acoustic period from  $t = 0$ . Wavelength and frequency are assumed for the waves at time  $t < 0$ . Chemical reactions begin to happen everywhere at time  $t = 0$ . The mean conditions would remain (nearly) spatially uniform at all times because the composition is initially uniform over the whole region and because the perturbations are considered to be minimal in relation to the corresponding mean quantities for the example under study. As shown in Fig. 1, any chemical effects on sound propagation would then be the same everywhere and would not cause a change in wavelength. Effects on amplitude and propagation speed or frequency, however, would rely on time rather than space.

The conservation equations of mass, momentum, and energy governing the unsteady, one-dimensional problem as represented by the model.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0 \dots\dots\dots 1$$

$$\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) + \frac{\partial p}{\partial x} = 0 \dots\dots\dots 2$$

$$\rho c_p \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) - \frac{\partial p}{\partial t} - u \frac{\partial p}{\partial x} - \omega H = 0 \dots\dots\dots 3$$

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Assume that all quantities such as pressure, temperature, etc., can be split into a mean and a fluctuating part, so that, for example,

$$T = \bar{T} + T', \tag{4}$$

The following equations for the fluctuating quantities may be obtained by further noting that the medium is initially and consistently remains spatially uniform on average, and that the mean density is constant due to mass conservation for zero mean velocity.

$$\frac{\partial \rho'}{\partial t} + \bar{\rho} \frac{\partial u'}{\partial x} = 0 \tag{5}$$

$$\bar{\rho} \frac{\partial u'}{\partial t} + \frac{\partial p'}{\partial x} = 0 \tag{6}$$

$$\bar{\rho} c_p \frac{\partial T'}{\partial t} + \rho' c_p \frac{d\bar{T}}{dt} - \frac{\partial p'}{\partial t} - w'H = 0 \tag{7}$$

For a perfect gas with constant specific heats, Eq. (5) and (7) can be combined to yield the following.

$$\frac{\partial p'}{\partial t} + \gamma \bar{p} \frac{\partial u'}{\partial x} = (\gamma - 1) w'H \tag{8}$$

$$u' = \frac{\partial \phi}{\partial x} \quad \text{and} \quad p' = - \bar{p} \frac{\partial \phi}{\partial t} \tag{9}$$

$$\frac{\partial^2 \phi}{\partial t^2} - \bar{a}_s^2 \frac{\partial^2 \phi}{\partial x^2} = - \frac{(\gamma - 1)}{\bar{\rho}} w'H \tag{10}$$

where  $\bar{a}_s^2$ , equal to  $\gamma RT$  or  $\gamma p/\rho$ , is the mean of the square of the isentropic frozen sound speed.

Equation (10) is similar to the classical acoustic equation, except for the following differences: Due to temporal change in the mean conditions resulting from chemical reaction,  $\bar{a}_s^2$  is a function of time through temperature or pressure variation. (b) There is a source term on the right-hand side of the equation, due to fluctuations in the reaction rate resulting from the acoustit: waves.

Consequently, it may be said that there can be a coupling between chemical kinetics and sound propagation. The linked effects will be discovered to have distinct qualitative characteristics for exothermic and endothermic

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processes, and to rely on activation energy, enthalpy of reaction, and ratio of chemical to acoustic time in the discussion that follows.

**Chemical and Acoustic Time.**

As was said in the preceding discussion, there are two distinctive times that are important in this particular case. The acoustic time, which is inversely related to the acoustic frequency, is undoubtedly one of these periods. The other one gauges the speed of a chemical reaction and can be described as follows in one form:

By the use of that part of Eq. (3) to be satisfied by the mean quantities, one can easily show that

$$\bar{\tau} \equiv \frac{\bar{T}}{d\bar{T}/dt} \dots\dots\dots 11$$

$$\bar{\tau} = \frac{1}{\gamma} \left( \frac{\bar{p}}{\bar{w}} \right) \left( \frac{c_p \bar{T}}{H} \right) \dots\dots\dots 12$$

Thus,  $\bar{\tau}$  represents a characteristic reaction time,  $T/T$ , modified by all enthalpy ratio,  $cpT/H$ , and the 'ratio of specific heats,

One can overlook effects caused by gradual changes in the mean circumstances during an acoustic period when the chemical time is longer than the acoustic time. The primary causes of these effects, as indicated by the right-hand side of Eq. (10), are variations in the response rate. Let the reaction rate  $w$  at temperature  $T$  be represented by the following expression; viz

$$w = \bar{w}_o (T/\bar{T}_o)^n \dots\dots\dots 13$$

Where the exponent  $n$  is a measure of the activation energy, with a large positive value of  $n$  representing high activation energy. Then,

$$\bar{w} = \bar{w}_o (\bar{T}/\bar{T}_o)^n \quad \text{and} \quad w' = n\bar{w} (T'/\bar{T}) \dots\dots\dots 14$$

Substituting Eq. (14) into Eq. (10) and employing the perfect-gas equation, one can obtain the following equation for the quasisteady case:

$$\frac{\bar{\tau}}{n} \frac{\partial}{\partial t} \left( \frac{\partial^2 \phi}{\partial t^2} - \frac{\bar{a}_s^2}{\gamma} \frac{\partial^2 \phi}{\partial x^2} \right) - \left( \frac{\partial^2 \phi}{\partial t^2} - \frac{\bar{a}_s^2}{\gamma} \frac{\partial^2 \phi}{\partial x^2} \right) = 0 \dots\dots\dots 15$$

Nondimensionalizing by the use of the instantaneous quantities, such that

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$$\bar{\phi} \equiv \omega_r \phi / R\bar{T} ,$$

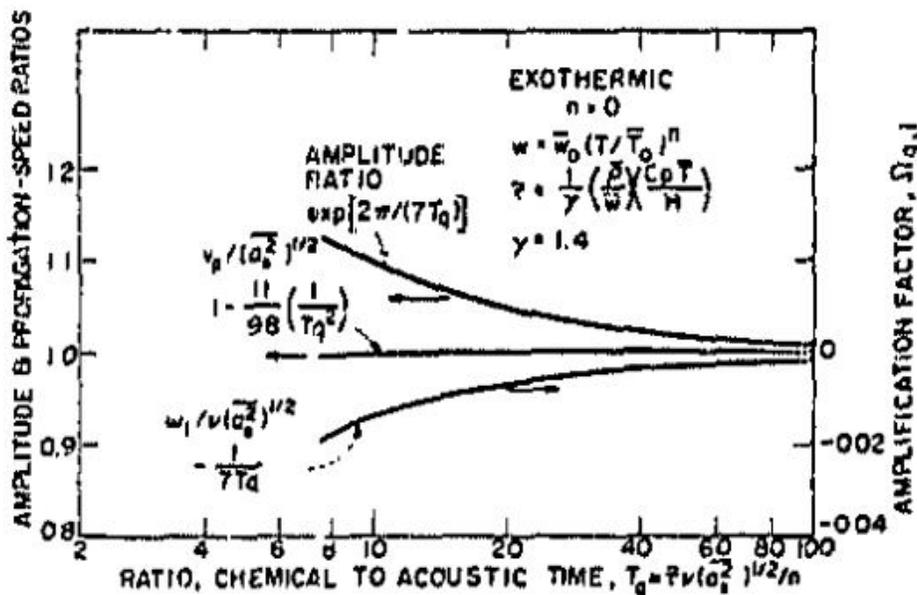
$$\bar{x} \equiv \omega_r x / [a_s^2]^{1/2} \quad \text{and} \quad \bar{t} \equiv \omega_r t \quad \dots\dots\dots 16$$

$$\frac{\bar{\omega}_r}{n} \frac{\partial}{\partial \bar{t}} \left( \frac{\partial^2 \bar{\phi}}{\partial \bar{t}^2} - \frac{\partial^2 \bar{\phi}}{\partial \bar{x}^2} \right) - \left( \frac{\partial^2 \bar{\phi}}{\partial \bar{t}^2} - \frac{1}{\gamma} \frac{\partial^2 \bar{\phi}}{\partial \bar{x}^2} \right) = 0 \quad \dots\dots\dots 17$$

When considering the preceding equation, a few observations are pertinent. First, the sound propagation speed is almost equivalent to the frozen isentropic sound speed under the conditions for which the equation is valid, i.e., at high acoustic frequencies, to, to, to, n >> 1), since the components in the second parenthesis will be very small. Second, attenuation occurs for negative values of n, although amplification of acoustic waves is feasible for positive values. As a result, for positive n, endothermic reactions would exhibit attenuation while exothermic reactions would exhibit amplification (or WH > 0). Additionally, if n is zero—the point at which the reaction rate becomes independent of temperature—no chemical impact is anticipated. Thirdly, because Fo is present in Eq. (17), the chemical action is frequency dependent.

(Note that, aside from an extra "actor 3," in this instance, this 0.imensionless ratio is comparable to the Damk6hle.,'s third s,~mil~2i~y parameter.)

Referring to the model shown in Fig. 1, one may assume a solution for the potential function of the following form:



Chemical effects on sound propagation speed, amplification factor and amplitude ratio in one acoustic period, at different ratios of chemical to acoustic time-quasisteady case.

$$\phi = \phi_0 \exp[-i(\nu x - \omega t)] \quad \dots\dots\dots 18$$

$$\omega = \omega_r + i\omega_i \quad \text{and} \quad \nu = 2\pi/\lambda \quad \dots\dots\dots 19$$

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$$\begin{aligned}
 &(3\Omega_{q,r}^2 - \Omega_{q,i}^2 - 1)\Omega_{q,i}T_q \\
 &\quad + (\Omega_{q,r}^2 - \Omega_{q,i}^2 - 1/\gamma) = 0 \\
 &(3\Omega_{q,i}^2 - \Omega_{q,r}^2 + 1)T_q + 2\Omega_{q,i} = 0 \dots\dots\dots 20
 \end{aligned}$$

$$\begin{aligned}
 \Omega_{q,r} &\equiv \omega_r/\nu(\bar{a}_s^2)^{1/2}, \\
 \Omega_{q,i} &\equiv \omega_i/\nu(\bar{a}_s^2)^{1/2}, \quad T_q \equiv \bar{\tau}\nu(\bar{a}_s^2)^{1/2}/n, \dots\dots\dots 21
 \end{aligned}$$

the subscript q indicates quasisteady solutions. These solutions are shown in Fig. 2 and will be discussed in a subsequent section.

As indicated earlier, one of the two possible chemical effects is due to temporal change in the mean conditions resulting from chemical reaction. In order to study this effect, one sets w" equal to zero in Eq. (10). (For the assumed reaction-rate expression, Eq. (14), this corresponds to n = 0 or zero activation energy.) Thus, the chemical effect is solely due to the fact that Eq. (10) is time dependent through temperature variation in the medium as a result of chemical reaction.

Again referring to Fig. 1 and noting that, in an infinite medium, the wavelength or the wavenum. bet remains uniform everywhere and constant at all times, one assumes a solution as follows:

$$\phi = \phi_0 \exp[-i(\nu x - \int_0^t \omega(t) dt)] \dots\dots\dots 22$$

$$\begin{aligned}
 \frac{d\bar{\tau}}{dt} &= 1 - n \\
 &= 1, \text{ for } n = 0, \dots\dots\dots 23
 \end{aligned}$$

$$\frac{\bar{a}_s^2}{a_{s,0}^2} = \frac{\bar{T}}{T_0} = \frac{\bar{\tau}}{\tau_0} = 1 + \frac{t}{\tau_0} \dots\dots\dots 24$$

One obtains the following two simultaneous, first order, nonlinear differential equations:

$$\frac{d\Omega_{c,i}}{dT_c} = \Omega_{c,i}^2 - \Omega_{c,r}^2 + 1 + \frac{T_c}{\bar{\tau}_c \omega_{r,0}} \dots\dots\dots 25$$

$$\frac{d\Omega_{c,r}}{dT_c} = 2\Omega_{c,i}\Omega_c \dots\dots\dots 26$$

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$$\frac{\overline{a_s^2}}{a_{s,0}^2} = \frac{\overline{T}}{T_0} = \left(\frac{\overline{\tau}}{\tau_0}\right)^{1/(1-n)}$$

$$= \left[1 + (1-n) \left(\frac{T_g}{\tau_0 \omega_{r,0}}\right)\right]^{1/(1-n)} \dots\dots\dots 27$$

$$\frac{d\Omega_{g,r}}{dT_g} = n \left(\frac{\gamma-1}{\gamma}\right) \left(\frac{1}{\tau_0 \omega_{r,0}}\right), \text{ and } \frac{d\Omega_{g,i}}{dT_g} = 0 \dots\dots\dots 28$$

Again, note that the solutions depend on  $t_0, w_r$ , and also whether the reaction is exothermic or endothermic,

**DISCUSSION OF RESULTS**

Analyzing Eq. (10) reveals that there are two main types of chemical impacts on sound propagation: those originating from chemical reactions that alter mean conditions. Those due to fluctuations in reaction rate resulting from acoustic waves. In this section these coupled effects will be discussed, as related to activation energy, enthalpy of reaction (either exothermic or endothermic), and ratio of chemical to acoustic time. Chemical impacts on sound propagation speed and amplification factor for various levels of the ratio of instantaneous chemical time to a corresponding frozen isentropic acoustic time for exothermic processes (where  $n > 0$ ) and  $\gamma = 1.4$ . The rms, instantaneous, frozen, isentropic, sound speed also serves as a normalization factor for the dimensionless propagation speed and amplification factor. The ratio of the amplitudes one acoustic period apart is also displayed in Fig. 2. In the case of exothermic, the amplitude grows over time. For endothermic processes, for which  $T_q$  is negative if  $n > 0$ , the same figure can be applied. Here, you can easily interpret the amplification factor as the appropriate damping factor (or  $flq.i > 0$ ) by taking its absolute value as the abscissa. As a result, the amplitude gets less with time. On the other hand, the propagation speed curve stays the same. The chemical influence on propagation speed is negligible inside the quasisteady analysis's validity range, as previously noted from Eq. (17) (as demonstrated by the approximate formulas in Fig. 2). With a 10% rise in amplitude (or 0.8 decibel) in one acoustic period with a value of 10 for  $T_q$ , for example, the influence on amplification or damping is not insignificant. It goes without saying that under these circumstances, the amplitudes would eventually grow to the point where nonlinear effects need to be taken into account. However, the chemical impact disappears as  $T_q$  approaches infinity.

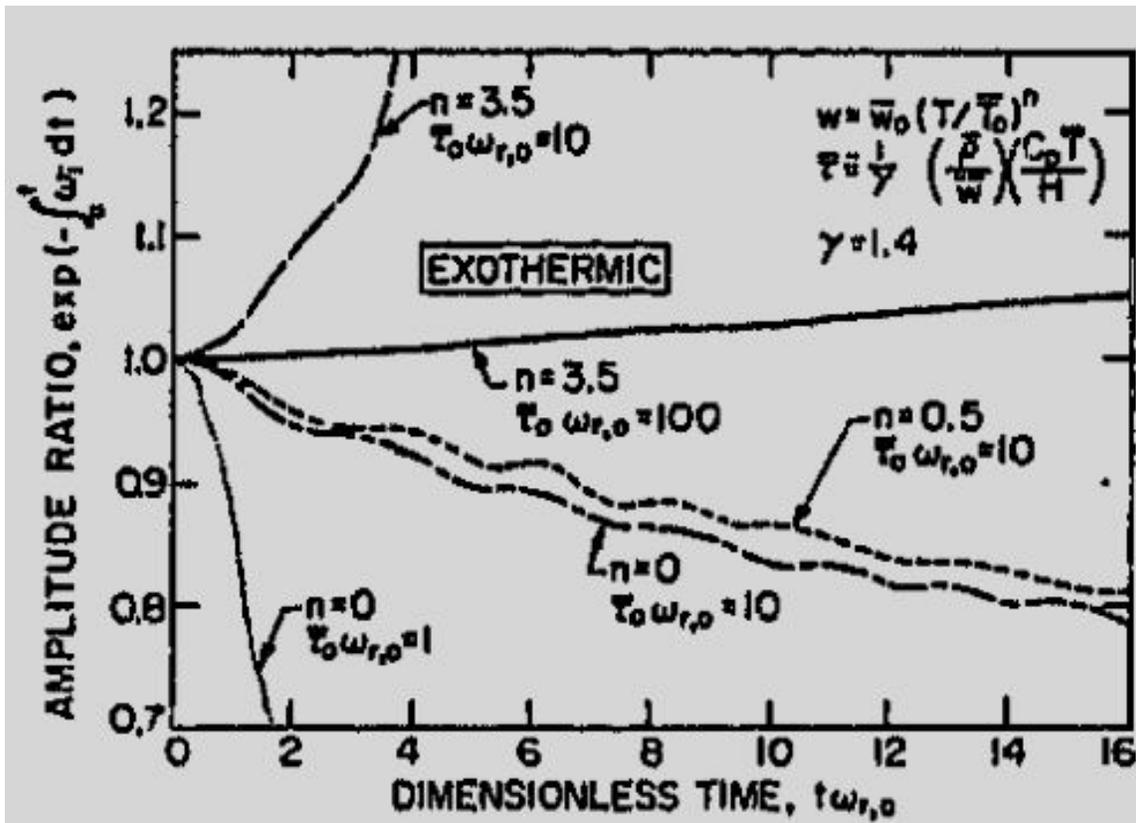
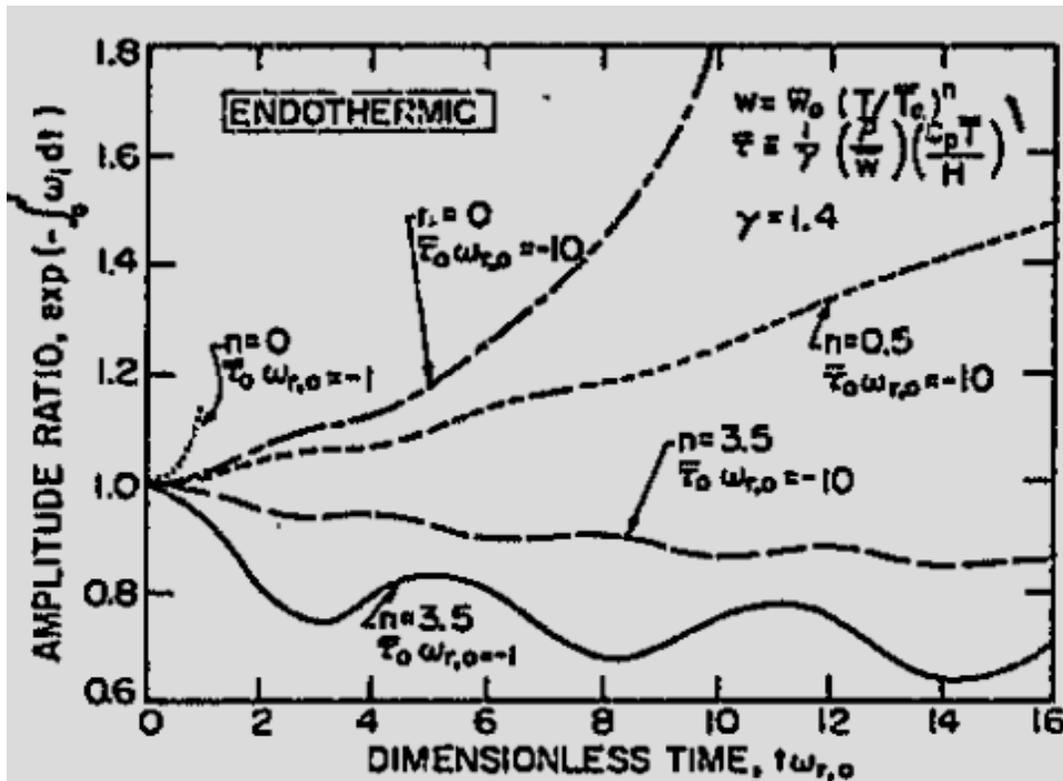


Fig. 3: temporal variation in amplitude for exothermic reactions, showing effects of temperature dependence of reaction rate and initial ratio of chemical to acoustic time.

Figures 3 and 4 show, respectively, for exothermic and endothermic reactions, temporal change  $t$  in amplitude for two absolute values each of the initial ratio of chemical to acoustic time; viz., 1 and 10. Contrary to what is predicted for the quasisteady case, the acoustic waves are here attenuated for exothermic reactions and amplified for endothermic reactions.

Additionally, there are variations in the change in amplitude. Observe also that the chemical impact increases in significance as the absolute value of  $\tau_0 \omega_{r,0}$  decreases, indicating the significance of the transitory chemical effect at relatively large reaction rates. Instantaneous propagation speed also fluctuates about the isentropic frozen sound speed. Again, for the sake of clarity such curves are not shown in Fig. 5 for  $n = 0$  (although curves for  $n = 3.5$  are included). In situations where temperature has no effect on reaction rate, the qualitative characteristics—namely, attenuation for exothermic reactions and amplification for endothermic reactions—are comparable to those seen in constant reaction rate reactions. Amplification for exothermic reactions and attenuation for endothermic reactions result from the reaction rate's greater temperature dependency at large activation energies ( $n = 3.5$ , for example), which also highlights the impacts of reaction rate variations. Naturally, these are the identical qualitative consequences as are anticipated for the quasisteady scenario, in which the only variations in reaction rate are the only source of chemical impact.



It is interesting to note that the activation energy and the enthalpy of reaction determine the initial rate of change in sound propagation speed with respect to the isentropic value. The behavior at higher activation energy and endothermic reaction is similar to that at low activation energy and exothermic reaction. Once more, this appears to correlate qualitatively with amplification effects.

### CONCLUSION

Chemical reactions and acoustic waves can cause mean condition changes and reaction rate variations, respectively, which can couple chemical kinetics and sound propagation. The propagation speed of a moving acoustic wave can alter as the reaction proceeds and can be amplified or dampened, depending on the activation energy, ratio of chemical to acoustic time, and whether the chemical reaction is exothermic or endothermic. Such coupling can in fact cause instability in responding medium under the right circumstances. When both kinds of chemical effects are considered, the results depend strongly on activation energy. For the case of small activation energy, where the reaction rate is weakly dependent on temperature, the qualitative effects are similar to those observed for constant reaction rate. For large activation energy, however, effects due to fluctuations in reaction rate become pronounced, leading to amplification for exothermic reactions and attenuation for endothermic reactions. In all cases, chemical effects become more significant at higher reaction rates.

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