

APPLICATION OF HEAT-BALANCE INTEGRAL METHOD TO CONJUGATE THERMAL EXPLOSION

by

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Conjugate thermal explosion is an extension of the classical theory, proposed and studied recently by the author.

The paper reports application of heat-balance integral method for developing phase portraits for systems undergoing conjugate thermal explosion. The heat-balance integral method is used as an averaging method reducing partial differential equation problem to the set of first-order ordinary differential equations. The latter reduced problem allows natural interpretation in appropriately chosen phase space.

It is shown that, with the help of heat-balance integral technique, conjugate thermal explosion problem can be described with a good accuracy by the set of non-linear first-order differential equations involving complex error function. Phase trajectories are presented for typical regimes emerging in conjugate thermal explosion.

Use of heat-balance integral as a spatial averaging method allows efficient description of system evolution to be developed.

Key words: thermal explosion, conjugate, heat balance integral method, phase portrait

Introduction

Thermal explosion theory is at foundation of combustion science, and has been an area of intensive research for over 80 years. It offers scientific basis for understanding of a vast range of phenomena occurring in industrial and safety applications. Derived first in 1928 by Semenov in his fundamental paper [1], critical conditions for thermal explosion were then considered in the framework of Frank-Kamenetskii theory [2]. The latter takes into account temperature distribution in the reaction zone by considering heat transfer equation with a non-linear (Arrhenius) chemical source term. Frank-Kamenetskii theory has become the most conventional formulation of the thermal explosion problem.

The exploration of thermal explosion theory has taken different routes since (see, for example [3-7]). There are two major directions which can be identified. These are kinetic and thermal lines of research. The first considers various effects of complicated chemical kinetics, such as different kinetic mechanisms, autocatalysis, parallel reactions, *etc.* The second direction investigates complicated forms of heat transfer within reacting mixture, as well as of thermal exchange between the mixture and its surroundings.

Conjugate thermal explosion is an extension of the classical theory proposed in the recent publication [8]. It involves multiple (two in the simplest form) chemically reacting media

which can thermally interact with each other. Critical conditions in such systems have been shown [8] to differ significantly from the classical one-media problem.

Heat-balance integral method (HBIM) is also a classical area of investigation in thermal science [9], which has been shown to be very successful for variety of problems. Obviously, practical importance of the method has diminished drastically from there it was fifty years ago due to revolution in scientific computation. However, the method is still quite popular and viable since its underlying philosophy is quite fundamental.

In the present paper, the method is applied to developing phase portraits of thermal system evolution. This is less traditional approach compared to approximate solution of unsteady heat transfer partial differential equations (PDE) for which the method has been originally developed. Although not entirely new (bits and pieces of similar philosophy can be traced through the literature), this interpretation of HBIM is rather fresh and the author is not immediately aware of the studies which were explicitly concerned with application of the HBIM for interpreting system evolution in the phase space.

The present paper merges therefore the two classical problems. Conjugate thermal explosion problem is investigated by application of HBIM as a spatial-averaging technique. This leaves one with the set of ordinary differential equations (ODE) whose interpretation on the phase plane provides quite accurate and concise picture of thermal system behavior.

Conjugate thermal explosion

For brevity, the problem is considered in the present paper for planar geometry. The development for the other two classical cases (*i. e.* cylindrical and spherical symmetries) can be performed in similar manner.

Extension of classical thermal explosion formulation [2] to the two slabs in thermal contact is as follows [8]:

$$\frac{\partial \theta_g}{\partial \tau} = \sqrt{t_{sg}^{ad}} \frac{1}{\delta_g} \frac{\partial^2 \theta_g}{\partial \xi^2} \exp(\theta_g), \quad 0 \leq \xi \leq 1 \quad (1)$$

$$\frac{d\theta_g}{d\xi} = 0, \quad \xi = 0 \quad (2)$$

$$\frac{\partial \theta_s}{\partial \tau} = \frac{1}{\sqrt{t_{sg}^{ad}}} \frac{1}{\delta_s} \frac{\partial^2 \theta_s}{\partial \zeta^2} \exp(\theta_s), \quad 1 \leq \zeta \leq \tilde{\zeta} \quad (3)$$

$$\frac{\partial \theta_s}{\partial \zeta} = \text{Bi} \theta_s(\tilde{\zeta}), \quad \zeta = \tilde{\zeta} \quad (4)$$

$$\theta_g = \theta_s, \quad \xi = \zeta = 1 \quad (5)$$

$$\frac{d\theta_g}{d\xi} = \lambda_{sg} \frac{d\theta_s}{d\zeta}, \quad \xi = \zeta = 1 \quad (6)$$

Boundary conditions (2) and (4) are the symmetry condition and the Newton-type heat exchange with surroundings, respectively. The last two equations are conditions at the interface, $\lambda_{sg} = \lambda_s / \lambda_g$ being the ratio between thermal conductivities of solid and gas media. Biot number is defined as $\text{Bi} = h_s r_s / \lambda_s$ where h_s is the convective heat transfer coefficient at the outer boundary and r_s is the transversal dimension of the solid region, respectively.

Conventional non-dimensional variables [3] are used here for the excess temperature θ , spatial coordinates ξ and ζ , and Frank-Kamenetskii parameters δ_g and δ_s . In general, adiabatic time scales [3] are different between the phases. A uniform non-dimensional time for the composite sample may be introduced as $\tau = t(t_g^{ad} t_s^{ad})^{-1/2}$, where t_g^{ad} and t_s^{ad} are adiabatic time scales for the corresponding phases. Note that the adiabatic time scale and Frank-Kamenetskii parameter may generally vary independently.

Conduction is assumed to be the only mode of heat transfer. For convenience of referencing, the material extending from $\xi = 0$ to $\xi = 1$ is called “gas”, and the one extending from $\zeta = \tilde{\zeta}$ “solid”, although the nature of materials may be arbitrary.

Critical conditions for conjugate thermal explosion with three different types of symmetry are reported in [8], where some numerical results are also presented.

Heat-balance integral formulation

Based on qualitative understanding of the process, and also typical results of numerical simulations [8], parabolic profiles are assumed for the two materials.

The natural characteristic points that can be chosen to characterize the process are the centerline of the vessel and the materials interface. This choice is justified by the observation that in most cases the explosion (thermal runaway) develops at the symmetry axis ($\xi = 0$). In some cases, runaway is also possible in the outer region, in which case it develops close to the interface between the two materials ($\xi = \zeta = 1$). Therefore, the centerline and material interface temperatures are convenient measures of the process development. They not only indicate the onset of thermal explosion, but also its location (inner or outer region).

The assumed profiles are chosen therefore as:

$$\begin{aligned} \theta_g(\xi, \tau) &= a_0(\tau) + a_1(\tau)\xi + a_2(\tau)\xi^2 \\ \theta_s(\zeta, \tau) &= b_0(\tau) + b_1(\tau)(\zeta - 1) + b_2(\tau)(\zeta^2 - 1) \end{aligned} \tag{7}$$

In this form, $a_0(\tau) = \theta_g(0, \tau)$ and $b_0(\tau) = \theta_s(1, \tau)$ are the temperature values at the center of the vessel and at the interface, which need be solved for.

Boundary and interface conditions (2, 4-6) are used to eliminate from (7) all the parameters except a_0 and b_0 :

$$\begin{aligned} \theta_g(\xi, \tau) &= a_0(\tau) + [a_1(\tau) + b_0(\tau)]\xi^2, \quad 0 \leq \xi \leq 1 \\ \theta_s(\zeta, \tau) &= b_0(\tau) + [f_1^1 a_0(\tau) + f_1^2 b_0(\tau)](\zeta - 1) \\ &+ [f_2^1 a_0(\tau) + f_2^2 b_0(\tau)](\zeta^2 - 1), \quad 1 \leq \zeta \leq \tilde{\zeta} \end{aligned} \tag{8}$$

Formulas for the coefficients f_i^j are provided in the Appendix.

The evolution equations for $a_0(\tau)$ and $b_0(\tau)$ are established by application of the HBI method itself:

$$\begin{aligned} \frac{\partial}{\partial \tau} \int_0^1 \theta_g(\xi, \tau) d\xi &= \sqrt{t_{sg}^{ad}} \left. \frac{1}{\delta_g} \frac{\partial \theta_g}{\partial \xi} \right|_0^1 - \int_0^1 \exp[\theta_g(\xi, \tau)] d\xi \\ \frac{\partial}{\partial \tau} \int_1^{\tilde{\zeta}} \theta_s(\zeta, \tau) d\zeta &= \sqrt{t_{sg}^{ad}} \left. \frac{1}{\delta_s} \frac{\partial \theta_s}{\partial \zeta} \right|_1^{\tilde{\zeta}} - \int_1^{\tilde{\zeta}} \exp[\theta_s(\zeta, \tau)] d\zeta \end{aligned} \tag{9}$$

Manipulation of eqs. (9) is rather tedious, and only the final result is retained here:

$$\begin{aligned}
 & \frac{da_0(\tau)}{d\tau} \frac{6\sqrt{t_{sg}^{ad}}}{\delta_g} \frac{g_2}{2g_2 g_1} [a_0(\tau) b_0(\tau)] \\
 & + \frac{3}{2} \sqrt{\pi} \sqrt{t_{sg}^{ad}} \frac{g_2}{2g_2 g_1} \sqrt{\frac{1}{a_a(\tau) b_0(\tau)}} \exp[a_0(\tau)] \operatorname{erf} \sqrt{a_0(\tau) b_0(\tau)} \\
 & \frac{1}{2g_2 g_1} \frac{1}{\sqrt{t_{sg}^{ad}}} \frac{1}{\delta_s} F[a_0(\tau), b_0(\tau)] G[a_0(\tau), b_0(\tau)] [\operatorname{Erfc}(\varphi_1) \operatorname{Erfc}(\varphi_2)] \\
 & \frac{db_0(\tau)}{d\tau} \frac{6\sqrt{t_{sg}^{ad}}}{\delta_g} \frac{g_1}{2g_2 g_1} [a_0(\tau) b_0(\tau)] \\
 & \frac{3}{2} \sqrt{\pi} \sqrt{t_{sg}^{ad}} \frac{g_1}{2g_2 g_1} \sqrt{\frac{1}{a_0(\tau) b_0(\tau)}} \exp[a_0(\tau)] \operatorname{erf} \sqrt{a_0(\tau) b_0(\tau)} \\
 & \frac{2}{2g_2 g_1} \frac{1}{\sqrt{t_{sg}^{ad}}} \frac{1}{\delta_s} F[a_0(\tau), b_0(\tau)] G[a_0(\tau), b_0(\tau)] [\operatorname{Erfc}(\varphi_1) \operatorname{Erfc}(\varphi_2)]
 \end{aligned} \tag{10}$$

The exact form of g_i , φ_i , $F(a_0, b_0)$, and $G(a_0, b_0)$, are again provided in the Appendix.

Note that final equations can be written conveniently and uniformly if complex error function is introduced. Depending on the signs of arguments, actual forms of RHSs in eqs. (10) may be different (but of course the resulting values are real in any case).

The RHSs of both equations look very similar, but in fact they are linearly independent. The reason for their similarity will be clear from the solution results, where in many cases $a_0(\tau)$ and $b_0(\tau)$ are seen as nearly proportional. However, there are sets of parameters for which this quasi-proportionality breaks down.

Results and discussion

Solutions $[a_0(\tau), b_0(\tau)]$ can be considered as a phase trajectories of the system in the phase space defined by the two characteristic temperatures a_0 and b_0 .

Numerical solutions of eqs. (10) are presented in figs. 1 and 2 for the two representative cases. Initially, the system is at the state $(a_0 = 0, b_0 = 0)$ at the bottom-left corner of the plots, and then progresses towards the upper-right corner as the time increases.

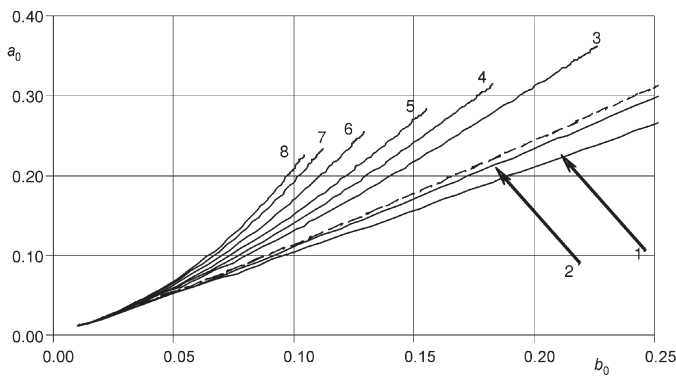
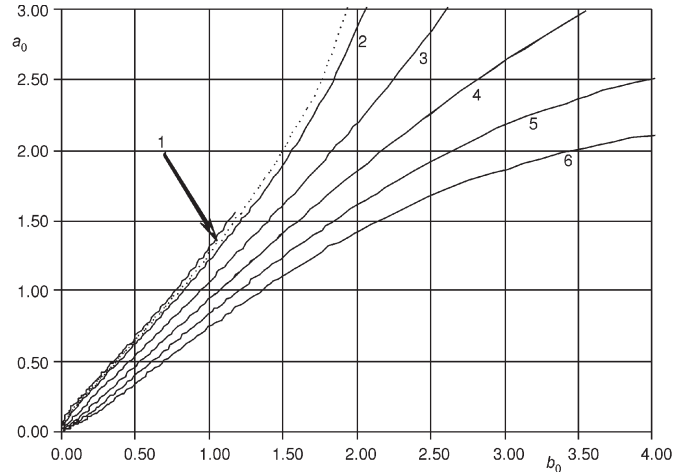


Figure 1. Phase portrait of the system for the case of explosion developing at the centre of the vessel; $\delta_g = 0.2$, $\delta_s = 0.2$, $\lambda_{sg} = 10.0$
 1 - $Bi = 0.1$, 2 - $Bi = 0.3$,
 3 - $Bi = 0.8$, 4 - $Bi = 1.0$,
 5 - $Bi = 1.2$, 6 - $Bi = 1.5$,
 7 - $Bi = 1.8$, 8 - $Bi = 2.0$
 Dashed line - separatrix

Figure 2. Phase portrait of the system for the case of explosion developing in the vicinity of material interface $\delta_g = 0.165$, $\lambda_{sg} = 2.65$, $Bi = 11.32$
 $1 - \delta_s = 12.48$, $2 - \delta_s = 24.96$,
 $3 - \delta_s = 49.92$, $4 - \delta_s = 74.88$,
 $5 - \delta_s = 99.84$, $6 - \delta_s = 124.80$
 Dashed line – separatrix



In the case shown in fig. 1, all the parameters are fixed except for the Biot number. The curves 1 and 2 represent the situations of thermal instability (explosion), and these curves can be extended indefinitely $[(a_0(\tau) \rightarrow \infty, b_0(\tau) \rightarrow \infty)]$. The rest of the curves (3-8) approach finite points asymptotically, and represent situations where thermal equilibrium is established. The separatrix, shown by the dashed line distinguishes “explosion – no explosion” behaviors and marks therefore the critical conditions (critical Bi number in this instance, since all the other parameters are fixed).

Explosion develops at the centre of the vessel for the case shown in fig. 1. This is seen from the fact that $a_0(\tau)$ becomes larger than $b_0(\tau)$ as temperature rise progresses (curves 1 and 2). This difference develops much more profoundly at later stages (see fig. 3 below).

Figure 2 illustrates different case where Frank-Kamenetskii parameter for the solid phase varies, rather than Biot number. Explosion occurs for high values of this parameter (curves 2-6). The only curve which represents existence of thermal equilibrium is the curve 1 ($\delta_s = 12.48$), just left from the separatrix. This curve approaches finite point asymptotically. Separatrix again marks critical conditions for the thermal explosion, this time in terms of minimum Frank-Kamenetskii parameter δ_s for the outer region.

Transition between two different types of explosion can be seen in fig. 2. For the curves 4, 5, and 6 in fig. 2, maximum temperature occurs in the outer region, since $b_0(\tau) > a_0(\tau)$ as $\tau \rightarrow \infty$. This type of behavior turns back to situation similar to fig. 1 (maximum temperature developing at the center) if parameter δ_s decreases (curves 2 and 3 in fig. 2).

Figures 1 and 2 illustrate therefore the two different regimes of conjugate thermal explosion development, *i. e.* explosion at the symmetry plane (centre of the vessel) or in the vicinity of the boundary between the two materials. Critical conditions for explosion are predicted by the HBI method to within 8% of their “exact” values, which can be obtained by solving numerically the full PDE problem.

For convenience, fig. 3 and 4 illustrate the same processes as figs. 1 and 2 by solutions of the exact PDE problem (1-6). The difference in temperature profile shapes during explosion phase is apparent.

The results show that HBI method can be helpful in reducing dimension of the problem and thus allowing its investigation through established mathematical methods, for example qualitative theory of ODE. The system described in the present paper is rather simple, but more complicated systems may be analysed in a similar manner. This application of qualitative ODE

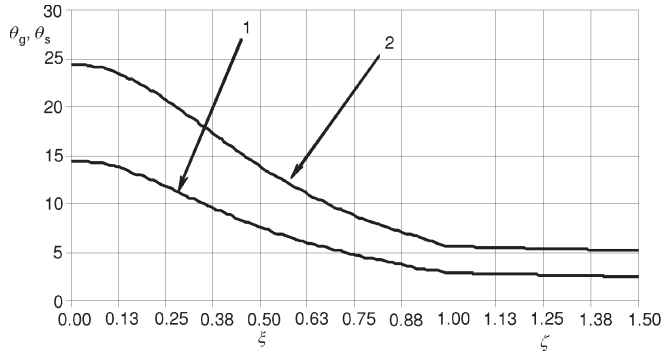


Figure 3. Detailed temperature profiles (PDE solution) illustrating explosion development for parameters δ_g , δ_s , and λ_{sg} , same as in fig. 1

1 – $Bi = 0.3$, $\tau = 1.05$, 2 – $Bi = 0.1$, $\tau = 1.05$

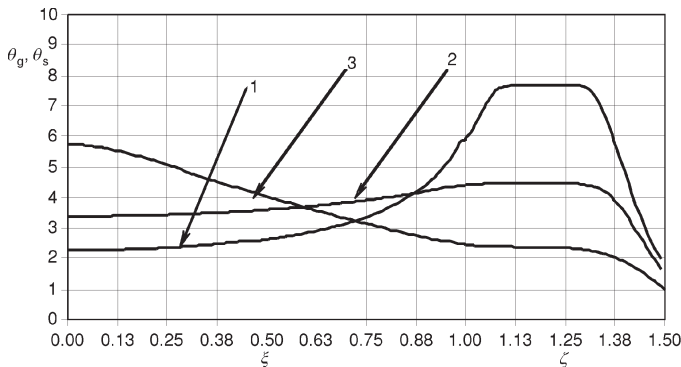


Figure 4. Detailed temperature profiles (PDE solution) illustrating explosion development for parameters δ_g , λ_{sg} , and Bi , same as in fig. 2

1 – $\delta_s = 124.80$, $\tau = 0.345$,
2 – $\delta_s = 74.88$, $\tau = 0.345$,
3 – $\delta_s = 24.96$, $\tau = 0.345$

methods (e. g. phase portraits and their transformation upon variation of parameters) will be quite helpful in interpretation of behavior of such complicated systems.

Conclusions

The present paper illustrates an application of HBI method to developing phase portraits of distributed thermal systems. The method is used as a kind of averaging method which allows simplified description of the systems in terms of first-order ODEs.

Recently proposed problem of conjugate thermal explosion serves as illustration. The problem has been shown to be reducible to the set of first-order ODEs involving complex error function.

The proposed application of HBI method as an averaging technique has a strong potential for investigation of complicated thermal systems.

Nomenclature

a_i, b_i – temperature profile coefficients, [–]
 Bi – Biot number, [–]
 t_{sg}^{ad} – adiabatic time ratio, [–]

ξ – spatial coordinate, [–]
 ζ – spatial coordinate, [–]
 ζ – spatial dimension of the media, [–]
 τ – time, [–]

Greek letters

δ – Frank-Kamenetskii parameter, [–]
 λ_{sg} – thermal conductivity ratio, [–]
 θ – excess temperature, [–]

Subscripts

g – gas
s – solid

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Appendix

This Appendix lists a variety of coefficients and functions met in the earlier formulas

$$f_1^1 = \frac{\text{Bi}(\tilde{\zeta}^2 - 1) - 2\tilde{\zeta}}{\lambda_{\text{sg}} \{(\tilde{\zeta} - 1)[\text{Bi}(\tilde{\zeta} - 1) - 2]\}}$$

$$f_1^2 = \frac{2 - \text{Bi}[(\tilde{\zeta}^2 - 1) - \lambda_{\text{sg}}] - 2\tilde{\zeta}}{\lambda_{\text{sg}} (\tilde{\zeta} - 1)[\text{Bi}(\tilde{\zeta} - 1) - 2]}$$

$$f_2^1 = \frac{\text{Bi}(\tilde{\zeta} - 1) - 1}{\lambda_{\text{sg}} \{(\tilde{\zeta} - 1)[\text{Bi}(\tilde{\zeta} - 1) - 2]\}}$$

$$f_2^2 = \frac{[\text{Bi}(\tilde{\zeta} - 1) - 1][(\tilde{\zeta} - 1)\{[\lambda_{\text{sg}} - 2(\tilde{\zeta} - 1)]\text{Bi}(\tilde{\zeta} - 1) - \lambda_{\text{sg}}\text{Bi}(\tilde{\zeta} - 1)\}]}{\lambda_{\text{sg}} \{[\text{Bi}(\tilde{\zeta}^2 - 1) - 2\tilde{\zeta}][(\tilde{\zeta} - 1)[\text{Bi}(\tilde{\zeta} - 1) - 2]\}}$$

$$g_1 = \frac{1}{2}(\tilde{\zeta} - 1)^2 f_1^1 - \frac{1}{3}(\tilde{\zeta}^3 - 1) - (\tilde{\zeta} - 1) f_2^1$$

$$g_2 = (\tilde{\zeta} - 1) \frac{1}{2}(\tilde{\zeta} - 1)^2 f_1^2 - \frac{1}{3}(\tilde{\zeta}^3 - 1) - (\tilde{\zeta} - 1) f_2^2$$

$$\varphi_1 = i \sqrt{f_2^1 a_0(\tau) - f_2^2 b_0(\tau)} \frac{1}{2} \frac{f_1^1 a_0(\tau) - f_1^2 b_0(\tau)}{\sqrt{f_2^1 a_0(\tau) - f_2^2 b_0(\tau)}}$$

$$\varphi_2 = i \sqrt{f_2^1 a_0(\tau) - f_2^2 b_0(\tau)} \tilde{\zeta} \frac{1}{2} \frac{f_1^1 a_0(\tau) - f_1^2 b_0(\tau)}{\sqrt{f_2^1 a_0(\tau) - f_2^2 b_0(\tau)}}$$

$$F[a_0(\tau), b_0(\tau)] = [(\tilde{\zeta} - 1)f_1^1 - (\tilde{\zeta}^2 - 1)f_2^1]a_0(\tau) + [(\tilde{\zeta} - 1)f_1^2 - (\tilde{\zeta}^2 - 1)f_2^2 - (1 - Bi)]b_0(\tau)$$

$$G[a_0(\tau), b_0(\tau)] = i \frac{\exp\left(\frac{f_1^1 - f_2^1}{f_1^2 - f_2^2} a_0(\tau) + \frac{f_1^2 - f_2^2 - 1}{f_1^2 - f_2^2} b_0(\tau)\right) \frac{1}{4} \frac{[f_1^1 a_0(\tau) - f_1^2 b_0(\tau)]^2}{f_2^1 a_0(\tau) - f_2^2 b_0(\tau)}}{\sqrt{f_2^1 a_0(\tau) - f_2^2 b_0(\tau)}}$$

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