

## MODELING OF SANDWICH HETEROGENEOUS PROPELLANT WITH TWO STEPS CHEMICAL KINETICS AND FLUID MECHANICAL EFFECTS

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### ABSTRACT

The numerical procedure for the burning of Ammonium Perchlorate (AP) with a Fuel-Binder (Hydroxyl Terminated Polybutadiene HTPB) is presented. This model accounts for the two-steps reaction mechanism for the primary diffusion flame between the decomposition products of the Binder (B) and the oxidizer AP and the primary premixed AP flame. Moreover, this current model allowed for the complete coupling between the gas-phase physics, the condensed-phase physics, and the unsteady non-uniform regression of the propellant surface. The parameters used in this model are fitted to experimental data for the combustion of AP/HTPB. The propagation of the unsteady non-planar regression surface is described, using the Essentially-Non-Oscillatory (ENO) scheme with the aid of the level set strategy. The Alternating-Direction-Implicit (ADI) solver is employed to solve the full Navier-Stokes equations in the gas phase for the variable density model. The results show the effect of various parameters on the surface propagation speed, flame structure, and the burning surface geometry. A comparison between the computational and experimental results is presented.

يتناول هذا البحث عمل نموذج لاحتراق عينة صغيرة من الوقود الصلب المستخدم في محركات الصواريخ على قدر صغر طبقة الاحتراق كمشكلة للوصول لأداء نموذج يشتمل على شتى أنواع اللهب المحتملة. وينفرد هذا البحث بالأخذ في الاعتبار تفاعل كيميائي ثنائي الخطوة يشتمل على اللهب الناتج من المؤكسد والمتكون فوقه ملاصقا لسطح الاحتراق والأصعب تطبيقه نظريا لأنه يحتاج لمعالجات خاصة بتركيز شبكات الحل العددية بشكل مكثف بجوار سطح الاحتراق حتى يصور التفاصيل الكاملة للهب علاوة على الصعوبات الناشئة عن حركة سطح الاحتراق المتغير مع المسافة والزمن والتي تحتاج أيضا إلى تحويل في معادلات الحركة. واللب الثاني المنتشر عند منطقة إنتقاء الوقود بالمؤكسد. وقد استخدم نموذج الساندوتش وهو عبارة عن شريحة من الوقود محاطة من كلا الجانبين بالمؤكسد. وقد بنيت الدراسة على حلول آتية باستخدام الطرق العددية لمعادلات الحركة في كل من جانب طور الغاز و جانب طور الوقود الصلب وكذا سطح الاحتراق المتحرك بينهما والمتغير مع المسافة والزمن في هذا النموذج. ويهدف هذا البحث لدراسة تأثير المتغيرات المختلفة للغازات المنطلقة داخل غرفة الاحتراق من هذه الأنواع من اللهب على شكل سطح ومعدل الاحتراق.

**Keywords:** Solid rocket propellants , Moving interfaces, Level set method, sandwich propellant, AP/HTPB.

### 1. INTRODUCTION

The complex flame structure that is generated by burning of a heterogeneous solid rocket propellant is proposed by Beckstead, Derr, and Price (the BDP model) [1]. Three separate flames can be identified in the gas phase. The first one is the primary flame between the decomposition products of the binder and the oxidizer. The second one is premixed oxidizer flame, while the third one is the final diffusion flame between the products of the other two flames. In spite of the BDP model is one-dimensional and necessarily omits or fails to properly account for important physics, but attempts to account for many of the significant feature of the combustion field. The influence of this work still endures [2], and 1D models are still used [3]. Several improvements to

BDP model of steady-state burning have been conducted. Lee et. al. [4] presented a modified picture for the flame structure for AP-HTPB-AP sandwich as shown in Fig.1. This sketch shows the principles of the combustion zone, in which the oxidizer-fuel flames consists of a Leading-Edge Flame (LEF) that stands in the mixing region of the oxidizer and fuel vapors, and a diffusion flame that trails from the LEF up to a point where the fuel vapor is all consumed. The LEF is a region of very high heat release as compared to the rest of the diffusion flames and contributes most of the heat transfer back to the propellant surface. This edge occurs because the diffusion flame can not extend all the way to the surface, the temperature there being relatively low.

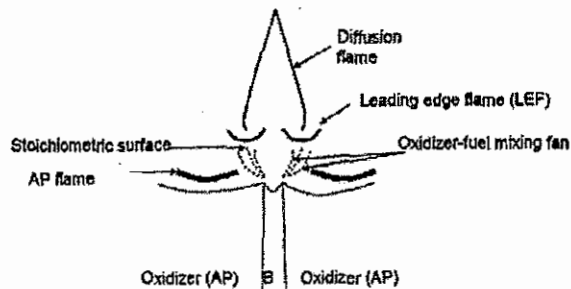


Fig. 1 Flame complex for an AP-Binder-AP sandwich [4]

The theoretical studies for the combustion of heterogeneous solid rocket propellant have faced a lot of difficulties because of the chemical and physical complexity of the propellant and the microscopic scale of the combustion zone. Therefore, few experimental studies have been performed for the simplest model of the combustion of Ammonium Perchlorate sandwiches [4,5]. The propellant was made from sheets of AP-HTPB-AP. The AP formed by dry pressing ultra pure AP powder. Observations for the combustion were made by high-speed camera and microscopic inspection of quenched samples. In addition, Lee et. al. [4] illustrated the effect of inclusion of particulate AP in the binder on the combustion surface and the flame structure. The effect of three types of fuel binder and oxidizer particle diameter on the decomposition and combustion behavior of ammonium perchlorate is studied by Al-Harathi and Williams, [6].

Few decades ago, several theoretical studies on the combustion field of the burning of the heterogeneous propellant have been conducted. These researches are divided into two main categories. The first one is concentrated on the gas phase modeling without consideration for the condensed phase process, for example [7,8,9,10,11]. The second one is studied the condensed phase reaction as the most important factor, for example [12,13]. Recently, several computational models [14,15,16 and 17] have been conducted to account the complex coupling between the solid-phase and gas-phase process. In particular, the complexity that arises from the consideration of the unsteady non-planar regression surfaces.

In the present paper a complete numerical method to examine what is perhaps, the simplest model is developed and account the following ingredients: the primary diffusion flame between the decomposition products of the binder and the oxidizer (AP), the primary premixed AP flame, different properties (density, conductivity) of the AP and binder, temperature-dependent gas-phase transport properties, an unsteady non-planar regression surface; and a proper accounting of the fluid-

mechanics in the gas-phase (retention of the Navier-Stokes equations). These ingredients are applied to the problem of Periodic Sandwich Propellant PSP (alternating slices of AP and binder).

## 2. The PHYSICAL AND MATHEMATICAL MODELS

The physical model of the PSP model is shown in Fig. 2. This model consists of a sheet of fuel-binder of thickness " $v$ ", layered between two sheets of ammonium perchlorate (AP). Above the solid surface is the gas phase, consisting of a mixture of the decomposition products of the solid oxidizer and fuel. Periodic boundary conditions are applied at  $x=\pm L$ . The AP-HTPB-AP sandwich geometry has been recognized as a useful framework to gain fundamental insights into propellant combustion (e.g. [16,17, and 18]) and a notable experimental program has been pursued for some years by Price and his colleagues [5]. In addition, combustion behavior of the simpler sandwiches is much easier to be observed and is enabled us to describe the combustion fields of the complex random packing propellant.

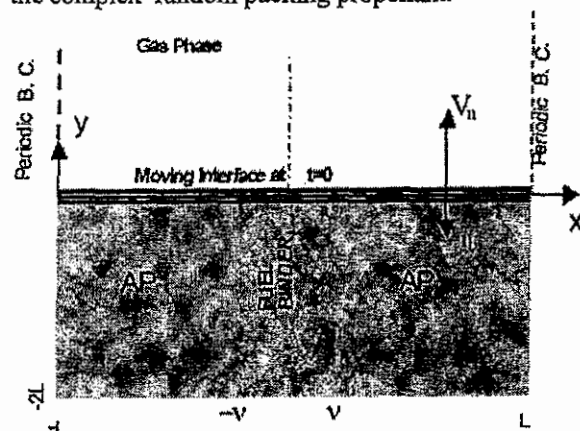
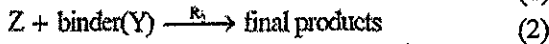
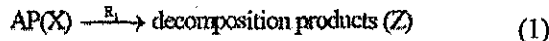


Fig. 2. Periodic sandwich propellant configuration

### 2.1. Constant and Variable Density Models

It is useful to summarize the formulation of the constant density model before addressing the complete problem, as this enable us to introduce most of the model ingredients together with various convenient scaling in the context of a model set of equations. The specific details of the constant density model for our problem are as follows: the density is set equal to constant (so that the equation of state, Charles law, is jettisoned); and a uniform velocity field  $u=0$  and  $v(y) = \text{constant}$  is adopted, which satisfies both the continuity and momentum equations. The one-step kinetics that include the primary flame is examined separately in order to achieve a good understanding of the unsteady burning of periodic sandwich propellant with complete coupling between the solid and gas phases. Thus;



$R_1$  and  $R_2$  are assumed to have the forms;

$$R_1 = B_1 P X \exp(-E_1/R_u T) \text{ and}$$

$$R_2 = B_2 P^{ng} Y Z \exp(-E_2/R_u T),$$

The corresponding gas phase equations are;

$$\rho_g \frac{D\phi}{Dt} = \vec{\nabla} \cdot \left( \frac{\lambda_g}{c_p} \vec{\nabla} \phi \right) + \Psi \quad (3)$$

where;  $\phi = [T \ X \ Y \ Z]^T$

$$\Psi = \left[ \frac{Q_{g1}R_1 + Q_{g2}R_2}{c_p} \ -R_1 \ -R_2 \ R_1 - \beta R_2 \right]^T$$

When full fluid-mechanics coupling (variable density model) is accounted for, the system of equations (3) is replaced by;

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = H \quad (4)$$

$$Q = \begin{bmatrix} \rho_g \\ \rho_g u \\ \rho_g v \\ \rho_g e \\ \rho_g X \\ \rho_g Y \\ \rho_g Z \end{bmatrix}; F = \begin{bmatrix} \rho_g u \\ \rho_g u^2 + P - \tau_{xx} \\ \rho_g uv - \tau_{xy} \\ (\rho_g e + P)u - (u\tau_{xx} + v\tau_{xy} - q_x) \\ \rho_g uX - \rho_g D_g X_x \\ \rho_g uY - \rho_g D_g Y_x \\ \rho_g uZ - \rho_g D_g Z_x \end{bmatrix};$$

$$G = \begin{bmatrix} \rho_g v \\ \rho_g vw - \tau_{xy} \\ \rho_g v^2 + P - \tau_{yy} \\ (\rho_g e + P)v - (u\tau_{xy} + v\tau_{yy} - q_y) \\ \rho_g vX - \rho_g D_g X_y \\ \rho_g vY - \rho_g D_g Y_y \\ \rho_g vZ - \rho_g D_g Z_y \end{bmatrix}; H = \begin{bmatrix} 0 \\ 0 \\ 0 \\ Q_g R_1 + Q_{g2} R_2 \\ -R_1 \\ -R_2 \\ +R_1 - \beta R_2 \end{bmatrix}$$

and;  $e = \frac{P}{\rho_g} + \frac{1}{2}(u^2 + v^2); \tau_{yy} = \mu \left( \frac{4}{3}v_y - \frac{2}{3}u_x \right);$

$$\tau_{xy} = \mu(v_x + u_y); \quad q_x = -\lambda_g T_x;$$

$$q_y = -\lambda_g T_y$$

Lewis number is taken to be unity, then;

$$\rho_g D_g = \lambda_g / c_p \quad (5)$$

With the aid of the equation of state;

$$P = \rho RT \quad (6)$$

where  $\beta$  is the stoichiometric ratio. Here there are six unknowns in the gas-phase, ( $u, v, T, X, Y, Z$ ) and one unknown in the solid-phase ( $T_s$ ).

### 2.2. Solid-Phase and Solid/Gas Interface Equations

In the solid-phase, the following heat equation is used;

$$\rho_s T_t = \frac{\lambda_s}{c_p} \nabla^2 T \quad (7)$$

The specific heat  $c_p$  is assumed to be equal to that in the gas phase for simplicity. The possibility of differing densities and thermal properties in the solid phase is allowed and setting by;

$$\rho_s = \begin{cases} \rho_{AP} & \psi \geq 0 \\ \rho_B & \psi < 0 \end{cases}; \lambda_s = \begin{cases} \lambda_{AP} & \psi \geq 0 \\ \lambda_B & \psi < 0 \end{cases} \quad (8)$$

The function  $\psi(x,y)$  is a level set function which demarks the regions of AP from binder (B) within the solid, so that a point  $(x,y)$  lies in the AP if  $\psi(x,y) \geq 0$ , and in the binder if  $\psi(x,y) < 0$ . Suppose the solid/gas interface defined by  $\eta(x(t),y(t),t) = 0$ . Then;

$$\eta_t + \eta_x \frac{dx}{dt} + \eta_y \frac{dy}{dt} = 0 \quad (9)$$

and the final equation that control the moving of the gas/solid interface as in Fig. 3 is derived by Hegab, et.al. [16,17] and may be written as follows;

$$\eta_t - r_b \left| \vec{\nabla} \eta \right| = 0, \quad (10)$$

where  $r_b$  is defined as the speed of the front which moves in the directions of the solid. In general  $r_b$  is given by the following simple pyrolysis law;

$$r_b = \begin{cases} r_{AP} = A_{AP} (P/P_0)^{n_{AP}} \exp\{-E_{AP}/R_u T_{AP,s}\} & \psi \geq 0 \\ r_B = A_B (P/P_0)^{n_B} \exp\{-E_B/R_u T_{B,s}\} & \psi < 0 \end{cases} \quad (11)$$

Note that pressure dependence has been added to the pyrolysis law for generality.

In the study, the propellant surface is not flat and its shape changes with time. Therefore, the following mapping function is used;

$$\eta = y - f(x,t) \quad (12)$$

and the the front of equation (10) reduces to the simple Hamilton-Jacobi equation;

$$f_t + r_b(x,t) \sqrt{1 + f_x^2} = 0, \quad (13)$$

Further information about the non-planar moving of the gas/solid interfaces using the Level Set strategy is mentioned in details in [16,17].

### 2.3. Boundary/Jump Conditions

The appropriate jump conditions  $[\phi]$  across the gas/solid interface are;

$$[\rho(\vec{v} \cdot \vec{n} + r_b)] = 0; \quad (14)$$

$$[T] = 0; \quad (15)$$

$$[\lambda \vec{n} \cdot \nabla T] = -Q_s m; \quad (16)$$

$$m [\chi_i] = [\rho D \bar{n} \cdot \nabla \chi_i], \quad i = 1, 2, 3, \quad (17)$$

where  $[\phi] = \phi_g - \phi_s$  denotes the jump in the quantity  $\phi$  across the interface,  $\chi_i$  refers to X, Y, and Z,  $m$  is the mass flux.  $\bar{n}$  is the unit normal pointing in the direction of the gas;  $\bar{n} = \nabla \eta / |\nabla \eta|$ , Fig. (3).  $Q_s$  is the solid phase heat release term defined by

$$Q_s = \begin{cases} Q_{AP} & \psi \geq 0 \\ Q_b & \psi \leq 0 \end{cases} \quad (18)$$

For an exothermic surface reaction,  $Q_s > 0$ , and for an endothermic reaction,  $Q_s < 0$ . Typically the AP is considered an exothermic reaction, while the binder is an endothermic one.

The recent studies by Hegab, et.al. [16,17] proved that the length and time scales for the front and the solid are the same order of magnitudes. On the other side, the ratio of the gas to solid or the ratio of the gas to front are of the order of  $10^{-3}$ . Thus for the present purpose, the quasi-steady approximation for the gas phase is employed. Note that disturbances with time scales of order  $10^{-3}$ s would effect the solid phase, but not the gas phase; changes on time scales of order  $10^{-5}$ s are needed to generate an unsteady gas phase and changes of this nature have been discussed in [11].

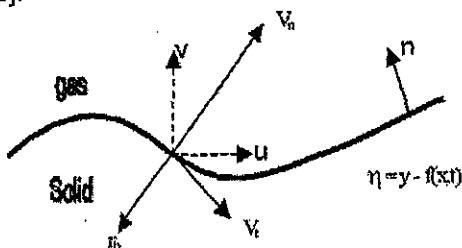


Fig. 3. Coordinate system for the moving surface

#### 2.4. Nondimensionalization

The following reference values is taken to nondimensionalize the equations ;

$$T^* = T/T_{ref}, \quad X^* = X/X_s, \quad Y^* = Y/Y_s, \quad Z^* = Z/Z_s, \quad P^* = P/P_0, \quad \rho^* = \rho/\rho_0,$$

$$(\dot{u}^*, \dot{v}^*) = (u, v)/V_g, \quad f^* = f/L, \quad \dot{r}_b^* = r_b/r_{b,ref}$$

$$(x^*, \eta^*) = (x, \eta)/L, \quad t^* = t/t_s, \quad t_s = L/r_{b,ref},$$

$$t_g = L/V_g, \quad \varepsilon = t_g/t_s \ll 1$$

$$V_g = \rho_{AP} r_{b,ref} / \rho_g, \quad T_{ref} = 2700 \text{ K}, \quad Q_{ref} = c_p * 2700 \text{ j/g}$$

Pressure  $p_0$  (bar), burning rate  $r_{b,ref}$  (cm/s), and mass flux  $m_{ref} = \rho_{AP} r_{b,ref}$ . Length  $L$  (half of the computational domain, which is the sum of the binder and the AP thickness). Time  $t = L/r_{b,ref}$ . Then the following non-dimensional parameters are defined: Peclet numbers  $Pe_g = \rho_g V_g L c_p / \lambda_{g,ref}$  and  $Pe_s = \rho_{AP} r_{b,ref} L c_p / \lambda_{AP}$ , Activation energy  $\theta = E/(R_u T_{ref})$

$$\hat{Q}_s = \begin{cases} Q_{s,AP} / (c_p T_{ref}) & \psi \geq 0 \\ Q_{s,B} / (c_p T_{ref}) & \psi < 0, \end{cases} \quad (19)$$

$$\lambda_{ratio} = \begin{cases} 1 & \psi \geq 0 \\ \lambda_B / \lambda_{AP} & \psi < 0, \end{cases} \quad (20)$$

$$\rho_{ratio} = \begin{cases} 1 & \psi \geq 0 \\ \rho_B / \rho_{AP} & \psi < 0. \end{cases} \quad (21)$$

In non-dimensional form the equations and boundary/connections form conditions are:

**For Constant Density Model**  $\eta > 0$

$$\varepsilon T_x^* + u T_x^* + v T_y^* = (1/P_e) \bar{\nabla} \cdot (\lambda \bar{\nabla} T) + Q_g R_1 + Q_g R_2$$

$$\varepsilon X_x^* + u X_x^* + v X_y^* = (1/P_e) \bar{\nabla} \cdot (\lambda \bar{\nabla} X) - R_1 \quad (22)$$

$$\varepsilon Y_x^* + u Y_x^* + v Y_y^* = (1/P_e) \bar{\nabla} \cdot (\lambda \bar{\nabla} Y) - R_2$$

$$\varepsilon Z_x^* + u Z_x^* + v Z_y^* = (1/P_e) \bar{\nabla} \cdot (\lambda \bar{\nabla} Z) + R_1 - \beta R_2$$

$R_1$  and  $R_2$  have the following forms;

$$R_1 = D_{a1} P X \exp(-\theta_{g1}/T)$$

$$R_2 = D_{a2} P^2 Y Z \exp(-\theta_{g2}/T),$$

but temperature-dependent transport is accounted for, viz;  $\lambda_g = \lambda_{g,ref} * \tilde{\lambda}(T, T_{ref})$  where  $\lambda_{g,ref}$  is a reference heat conduction coefficient. The value of  $\lambda$  at the reference temperature  $T_{ref}$ , specially  $\lambda_g = 1.08 * 10^{-4} T + 0.0133$  is choosing with dimensions W/m-K when T is assigned in degrees Kelvin, so that

$$\tilde{\lambda}(T, T_{ref}) = \frac{1.08 * 10^{-4} T_{ref} T + 0.0133}{1.08 * 10^{-4} T_{ref} + 0.0133} \quad (23)$$

$$u = 0, \quad v = -\rho_{ratio} f_t, \quad R = D_a P X Y \exp(-\theta_g/T) \quad (24)$$

**For Variable Density Model**  $\eta > 0$

The non-dimensional equations of motion can be rewritten in the following form:

$$\varepsilon \frac{\partial Q}{\partial t} + \frac{\partial F(Q)}{\partial x} + \frac{\partial G(Q)}{\partial y} = \frac{\partial V_1(Q, Q_x)}{\partial x} + \quad (25)$$

$$\frac{\partial V_2(Q, Q_y)}{\partial x} + \frac{\partial W_1(Q, Q_x)}{\partial y} + \frac{\partial W_2(Q, Q_y)}{\partial y} + H$$

$$\text{where, } Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \\ \rho X \\ \rho Y \\ \rho Z \end{bmatrix} \quad G(Q) = \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + \bar{p} \\ \rho v h \\ \rho v X \\ \rho v Y \\ \rho v Z \end{bmatrix}$$

$$V_1(Q, Q_x) = \begin{bmatrix} 0 \\ 4/3\alpha u_x \\ \alpha v_x \\ (\gamma-1)M^2\alpha\{4/3\alpha u_x + v v_x\} + \beta^* T_x \\ \mu/P_e X_x \\ \mu/P_e Y_x \\ \mu/P_e Z_x \end{bmatrix}$$

$$W_2(Q, Q_y) = \begin{bmatrix} 0 \\ \alpha u_x \\ 4/3\alpha v_x \\ (\gamma-1)M^2\alpha\{u u_y + 4/3\alpha v v_y\} + \beta^* T_y \\ \mu/P_e X_y \\ \mu/P_e Y_y \\ \mu/P_e Z_y \end{bmatrix}$$

$$V_2(Q, Q_y) = \begin{bmatrix} 0 \\ -2/3\alpha v_y \\ u_y \\ (\gamma-1)M^2\alpha\{-2/3\alpha v v_y + v u_y\} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$W_1(Q, Q_x) = \begin{bmatrix} 0 \\ \alpha v_x \\ -2/3\alpha u_x \\ (\gamma-1)M^2\alpha\{u v_x - 2/3\alpha v u_x\} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

where;  $\alpha = \frac{Sc}{P_e} \mu$ ,  $\beta^* = \frac{Sc}{P_e P_r} \lambda$ , and

$$h = e + \frac{\gamma-1}{\gamma} p / \rho$$

**For Solid Phase**  $\eta < 0$

$$\rho_{ratio}(T_t - f_t T_\eta) = (\lambda_{ratio} / P_{ec}) \Delta T \quad (26)$$

**For Moving Interface**  $\eta = 0$

$$f_t + r_b \sqrt{1 + f_x^2} = 0, \quad (27)$$

$$T(x, 0^+, t) = T(x, 0^-, t) \quad (28)$$

$$\hat{\lambda} \left( \frac{-f_x T_x + (1 + f_x^2) T_\eta}{\sqrt{1 + f_x^2}} \right) \Big|_{0^+} = -\hat{Q}_s m P_{e_s} \quad (29)$$

$$\hat{\lambda} \lambda_{ratio} \left( \frac{-f_x T_x + (1 + f_x^2) T_\eta}{\sqrt{1 + f_x^2}} \right) \Big|_{0^+} = -\hat{Q}_s m P_{e_s}$$

$$\left( mX - \frac{\hat{\lambda}}{P_{e_s}} \left[ \frac{-f_x X_x + (1 + f_x^2) X_\eta}{\sqrt{1 + f_x^2}} \right] \right) \Big|_{0^+} \quad (30)$$

$$= \begin{cases} m & \psi \geq 0 \\ 0 & \psi < 0 \end{cases}$$

$$\left( mY - \frac{\hat{\lambda}}{P_{e_s}} \left[ \frac{-f_x Y_x + (1 + f_x^2) Y_\eta}{\sqrt{1 + f_x^2}} \right] \right) \Big|_{0^+} \quad (31)$$

$$= \begin{cases} 0 & \psi \geq 0 \\ m & \psi < 0 \end{cases}$$

$$\left( mZ - \frac{\hat{\lambda}}{P_{e_s}} \left[ \frac{-f_x Z_x + (1 + f_x^2) Z_\eta}{\sqrt{1 + f_x^2}} \right] \right) \Big|_{0^+}$$

$$= \begin{cases} 0 & \psi \geq 0 \\ m & \psi < 0 \end{cases}$$

**For  $\eta \rightarrow \infty$**   $T = T_0$  (32)

**For  $\eta \rightarrow +\infty$**   $\frac{\partial}{\partial \eta} (\cdot) = 0$  (33)

For  $|x| = 1$  Periodic boundary condition (34)

### 3. NUMERICAL METHODS

#### 3.1. Modified Conservation Equations

To avoid pressure singularity at low Mach numbers, the numerical strategy outlines in [20] is used. The pressure is rescaled in the momentum equation since it is the pressure gradient, not the actual pressure, that is involved in the momentum balance. The rescaled pressure is applied to retain accuracy in calculating the momentum conservation. As a result, the pressure is divided into constant and fluctuating parts as follow;

$$P(x, y, t) = 1 + \gamma M^2 \hat{P}(x, y, t) \quad (35)$$

and substitute into the equations of motion given above. Where  $M$  is the Mach number ( $M = V_s / C_s$ ). The equation of state now becomes;

$$\rho = \frac{1 + \gamma M^2 \hat{P}(x, y, t)}{T} \quad (36)$$

and is used to update the density. Since the quasi-steady state solution in the gas phase ( $\epsilon \ll 1$ ) is required, the physical time term in Eqn.(25) is eliminated. In addition an accelerate convergence technique is employed [20]. The technique begins by adding a pseudo-time derivative to the conservation

equation (25). So the equations to be solved for the gas phase become;

$$\Gamma \frac{\partial \tilde{Q}}{\partial \tau} + \frac{\partial F(\tilde{Q})}{\partial x} + \frac{\partial G(\tilde{Q})}{\partial y} = \frac{\partial V_1(\tilde{Q}, Q_x)}{\partial x} + \frac{\partial V_2(\tilde{Q}, Q_y)}{\partial x} + \frac{\partial W_1(\tilde{Q}, Q_x)}{\partial y} + \frac{\partial W_2(\tilde{Q}, Q_y)}{\partial y} + H \quad (37)$$

where  $\tau$  represents the pseudo-time domain. Because the pseudo-time derivative vanishes at convergence to the steady state solution in the gas phase, a certain amount of liberty is given in choosing the variables in  $\tilde{Q}$ . A new scaled pressure term  $\tilde{P}/\beta$  is added as a pseudo-time derivative term to the continuity equation. The remaining variables in  $\tilde{Q}$  are then fixed by rewriting the momentum, energy, and species equations from their nonconservative form by means of the modified equation of mass conservation. As a result, the pseudo-time variable vector  $\tilde{Q}$  and its associated preconditioning matrix  $\Gamma$  takes the form;

$$\tilde{Q} = \begin{bmatrix} \tilde{P} \\ u \\ v \\ h \\ X \\ Y \\ Z \end{bmatrix}, \Gamma = \begin{bmatrix} 1/\beta' & 0 & 0 & 0 & 0 & 0 & 0 \\ u/\beta' & \rho & 0 & 0 & 0 & 0 & 0 \\ v/\beta' & 0 & \rho & 0 & 0 & 0 & 0 \\ h/\beta'-1 & 0 & 0 & \rho & 0 & 0 & 0 \\ X/\beta' & 0 & 0 & 0 & \rho & 0 & 0 \\ Y/\beta' & 0 & 0 & 0 & 0 & \rho & 0 \\ Z/\beta' & 0 & 0 & 0 & 0 & 0 & \rho \end{bmatrix} \quad (38)$$

Factor  $\beta'$  is used to properly scale the time derivative of  $\tilde{P}$ . Its selection is proportional to the dynamics pressure of the flow field.

### 3.2. ADI Algorithm Development

The first step for advancing the solution of (37) is using the Delta form scheme [19] as follows ;

$$\Delta Q^n = \frac{\theta \Delta \tau}{1+\xi} \frac{\partial}{\partial \tau} (\Delta Q^n) + \frac{\Delta \tau}{1+\xi} \frac{\partial}{\partial \tau} (Q^n) + \quad (39)$$

$$\frac{\xi}{1+\xi} \Delta Q^{n-1} + O\left[(\theta-1/2-\xi)\Delta\tau^2 + \Delta\tau^3\right]$$

$$\text{and } \Delta Q^n = Q^{n+1} - Q^n \quad (40)$$

The time-difference formulas (39) and (40), with the appropriate choice of the parameters  $\xi$  and  $\theta$  reproduce many familiar two and three level, implicit schemes. The three level, second order accuracy implicit schemes ( $\xi=1/2$  and  $\theta=1$ ) with special treatment for the cross derivative terms at the level (n-1) is applied. By inserting the temporal derivative of equation (37) in (39) and by straightforward derivation, the resulting approximated form can be splitted into two-tridiagonal systems;

$$\left[ I + \theta \Delta \tau \Gamma^{-1} \left( \frac{\partial}{\partial x} (A - P + R_x)^n - \frac{\partial^2}{\partial x^2} (R^n) \right) \right] \quad (41)$$

$$* \Delta Q^* = \Gamma^{-1} RHS$$

$$\left[ I + \theta \Delta \tau \Gamma^{-1} \left( \frac{\partial}{\partial y} (B - \tilde{Q} + S_y)^n - \frac{\partial^2}{\partial y^2} (S^n) \right) \right] \quad (42)$$

$$* \Delta Q = \Delta Q^*$$

where  $A^n, P^n, R^n, R_x^n, B^n, \tilde{Q}^n, S^n,$  and  $R_y^n$  are the jacobian matrices for the implicit x- and y-sweep (41,42) respectively. I is a unit matrix (6X6) and  $\Gamma^{-1}$  is the inverse of the preconditioning matrix.

The three-points second order accuracy central difference approximation are used for the spatial differences in the LHS of x-sweep form (41). This approximation along with the applied periodic boundary conditions at  $|x|=1$  produce a system of *Periodic Block-Tridiagonal Equations (PBTE)*. After the computation of  $\Delta Q^*$  at the interior points by solving this system of PBTE with each block having dimensions 6 x 6 components, the code is ready for the implicit y-sweep form (42). Here again, the three-points second order accuracy central difference approximation are used for the spatial differences in the LHS of (42). This approximation along with the rigid wall boundary conditions at  $y=0$  produce a system of *Non-Periodic Block-Tridiagonal Equations (NPBTE)*. The final delta form  $\Delta Q$  can be computed by solving the NPBTE system. Then the solution at new time step (n+1) can be determined from Eqn.(41). Note that, the cross-derivatives terms at (n-1) are treated explicitly to avoid the implicit coupling of adjacent boundary points.

The surface equation (13) is solved in order to follow the non-planar regression surface by the first order temporal scheme [22]. Beside the non-flat regression surface mapping as in (11), another transformation is applied for clustering grid points adjacent to the wall, where most of the flow parameters changes rapidly. The solution of the final mapped equations is advanced in the solid phase using physical time (t). Simultaneously the solution in the gas phase using pseudo-time ( $\tau$ ) to the local steady state at the first physical time step (t) is advanced. The boundary/jump conditions are continually updated as in Eqs. (26) to (34). Then the Hamilton-Jacobi Eqn. (13) is advanced at the physical time by a third order ENO and a fifth-order WENO (weighted essentially non-oscillatory) solver [23,24].

All numerical calculations were performed on a 140 x 70 grid, uniform in the x-direction and stretched in the y-direction. At each physical time, the solution in the gas phase is advanced until the relative difference between each two different pseudo-time values is less

than some prescribed tolerance, taken here to be  $10^{-6}$ . Convergence tests were carried out and it was determined that any further refinement resulted in less than 1% relative error.

#### 4. RESULTS AND DISCUSSIONS

The understanding of the complex combustion structure of AP-HTPB-AP sandwich, as a simple model to the heterogeneous solid rocket propellant, is studied in details by two different models. The first model is the constant density model and the second one is the variable density model or the Navier-Stokes model. Initially, the solution starts from a flat surface  $f(x,t=0)=0$ . Then the solution is advanced in the solid phase, gas phase with simultaneously moving interface. The first set of the results are for the constant density model. In this model, it has been taken  $\mu=\Lambda(T,T_{ref})$  which is one of the more realistic choices rather  $\mu=\text{constant}$  in earlier studies [7]. In the gas phase, the contours plots for the reaction rate contours (R) at different times are shown in figure (4) for  $\theta_{g1}=3.5$ ,  $\theta_{g2}=6.0$ ,  $\beta=7.51$ ,  $P_{eg}=6$ ,  $P_{1s}=2.9$ ,  $D_{a1}=5 \times 10^4$ ,  $D_{a2}=1.7 \times 10^5$ ,  $v=0.22$ ,  $Q_{g1}=0.833$ ,  $Q_{g2}=3.86$ ,  $Q_{s,AP}=-0.4$ , and  $Q_{s,B}=-0.06$ , as benchmark computation. The upper portion represents the gas phase and the lower one refers to the solid phase. The dark gray region in the latter represents the binder layer between the two AP sheets (light gray). The contour values are written in the upper part of each plot. The plot shows the location and shape of the generating flame. These reaction rate contours show a combined of two different flames. The first one is

the diffusion flame that formed at the interface between the oxidizer and the fuel, while the second one is the premixed flame that stands above the oxidizer regions. The contours of the diffusion flame show that reaction rate is characterized by two strong mixing structure each centered at  $|x|=0.223$ .

The successive curved shapes through the solid phase show that, the surface is initially flat and then as the solution is advanced, the combustion surface retreats in an unsteady fashion and finally retreats at a fixed speed with unchanged shape by  $t=2.49$ . These contours reveal not only the significant effect of the surface profiles and the burning rate on the shape of the flame but also on the maximum reaction rate values which decrease as time increase. The differences in profiles with time advanced reflect the behaviour of the burning rate at the propellant surface and reconstruct the corresponding flame structures and identify the parts of the flame structure that dominate the sandwich burning rate and the surface heat flux. In addition there is a sharp discontinuity in slope at the interface between the binder and AP regions. This interesting phenomena is predicted in [25].

Figure (5) shows a comparison between the experimental image for the structure of the flame shape and the burning surface (the left) [26] and the current computation model (the middle for the reaction rate and the right for the fuel vapour contours). The stoichiometric level surface shows the location at which the fuel and oxidizer meet together in stoichiometric proportions.

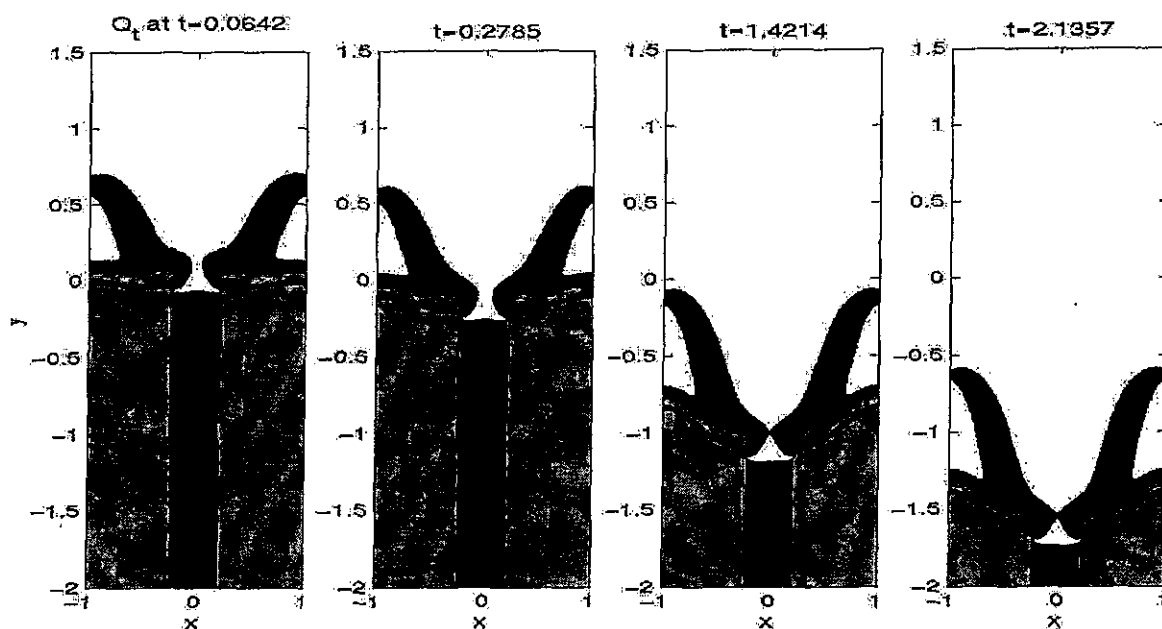


Fig. 4. Reaction rate contours at different times in the gas-phase for  $\theta_{g1}=3.5$ ,  $\theta_{g2}=6.0$ ,  $\beta=7.51$ ,  $P_{eg}=6$ ,  $P_{1s}=2.9$ ,  $D_{a1}=5 \times 10^4$ ,  $D_{a2}=1.7 \times 10^5$ ,  $v=0.22$ ,  $Q_{g1}=0.833$ ,  $Q_{g2}=3.86$ ,  $Q_{s,AP}=-0.4$ , and  $Q_{s,B}=-0.06$ .

The inner region for the stoichiometry contour is the fuel-rich region (see the fuel vapour image on the left side), while the area out of the stoichiometry envelop represent the fuel-lean composition. The two stoichiometric surface in both the computational and experimental images represent the two strong mixing structure (at the AP-Binder interface) each centered at  $|x| \sim 0.223$  and forming the flame envelop in addition to the AP-premixed flame that control the shape of the combustion surface above the AP region.

This comparison shows how the computational steadily surface regressing profile (at  $t > 5$ ) is qualitatively consistent with the experimental emission-transmission composite image by Brewster, et al. (2001), [26] and also with the experimental photography for the spontaneous quench samples of AP/BPAN/AP sandwich that reported by Lee et al. [4]. Both theoretical and experimental results verified that conditions that give the highest burning rates resulted in narrow smooth bands of binder in the middle with little "protrusion" of AP at the interface.

The variation of the burning rate  $C$  with the pressure is presented in figure (6) for the benchmark data as in Fig.(4). The response of the burning rate to the exposed pressure is one of the important and essential characteristics of the propellant. This figure shows that the burning rate is directly proportional to the pressure with exponential component about

( $n=0.6$ ). This exponential value has great interest to the rocket designer, in particular for the modeling of the composite propellant rather the sandwich one.

The effect of the exposed pressure on the burning surface profiles is presented in figure (7) at three pressure values  $P=1, 10, 15$  atm in the gas phase. A comparison between the experimental image and the computational model for the response of the combustion surface profiles to the pressure change (experimental at 7 atm in the left and the computational at 1, 10, and 15 atm in the right) is presented in figure(7). Both images illustrate that increasing the pressure causes the binder to stick out and the surface consist of a "trough" centered on the binder lamina. In addition a comparison of these clear pictures with the experimental results by Price et al. [5] is possible but caution is appropriate as the sandwiches that Price et al. examined are isolated, not periodic.

Furthermore, the effect of the pressure on the surface heat flux reveal that the heat flow vector, near the gas-solid interface and AP-binder solid interface, is from the binder toward the AP in the solid phase. Consequently there must exist a weak (hot) portion of the binder slightly up from the corner interface and into the binder. This might account for the appearance of the V-shape (notches) in the binder. This phenomena have been seen in the experimental quenched samples by Handley, et al. [25].

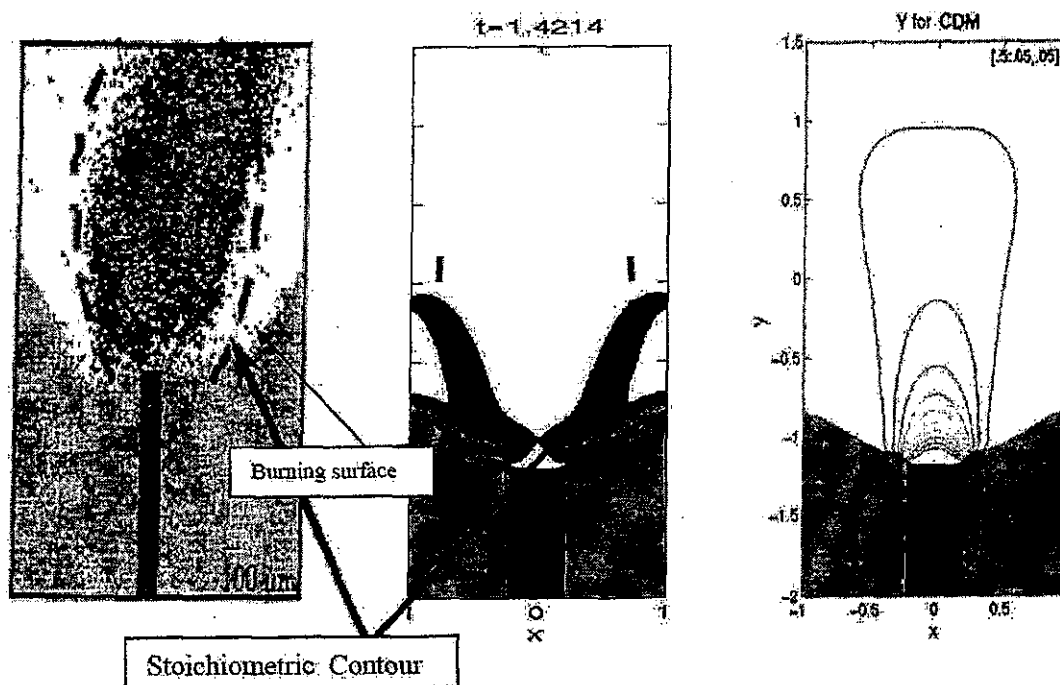


Fig. 5. Comparison of experimental image for the burning of AP-HTPB-AP sandwich[26] (left) with the numerical model (middle and right).



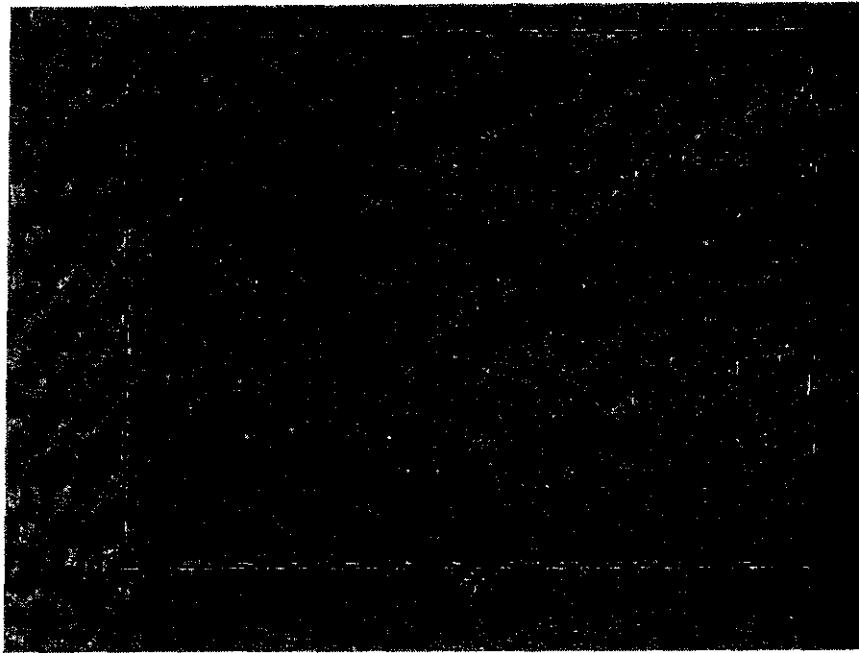


Fig. 6. Variations in the global regression rate with pressure.

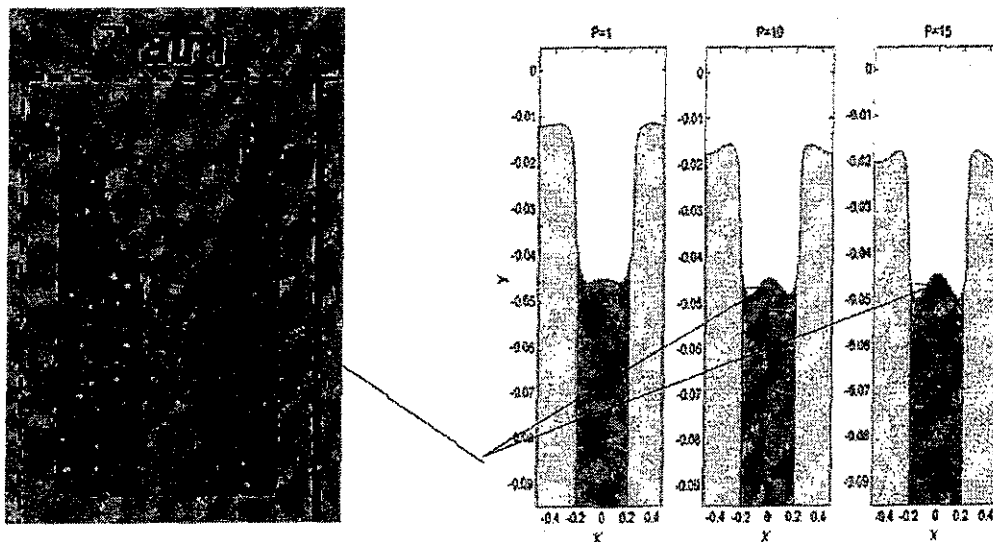


Fig. 7 Effect of pressure on the burning surface structure. Left figure is experimental [5] and the right figures are the present computational model.

The last set of the results are for the variable density model (2). In this section the results obtained from the constant density model(1) with those obtained using the Navier-Stokes equations, model(2) are compared, and thus to validate the simpler strategy. Figure(8) shows a comparison between the two models for the reaction rate contours for the parameters in Fig (4). The reaction rate values varied from 12 to 2 with incremental 2 for the AP-premixed flame, while varied from 1 to 0.2 with incremental 0.2 for the AP-Binder diffusion flame that centered near the interface between the fuel and oxidizer paused little bite toward the oxidizer surface. It is

noted that the flame is setting at the same transverse location with slight differences in the maximum reaction rate contours.  $RR_{max}$  is 11.88678 for model(2), compared to 11.66972 for model(1) and in the adiabatic flame temperature, where  $T'_{max}$  is 2448.09 K for model(2) compared to 2446.57 for model(1). These interesting values reveal that there is only a small difference in the far-field for the two models. These very slight differences are related to the slow flow accelerated since the axial velocity component  $u$  is not zero when the Navier-Stokes equations are used and the transverse velocity component becomes more or less in the

neighborhood of the flame for model(2). Figure(9) shows the axial velocity contours at different times for the Navier-Stokes model. It is noted that an axial velocity is generated near the combustion surface due to the surface morphology, where the velocity cells are positive on the left hand side, since the flow goes down hill and the right hand side cells are negative, since the flow goes up hill. Moreover, the absolute value of the axial velocity increases as time increases, since the curvature in the combustion surface profiles become more deeper than at earlier time.

The small differences between the two models reveal that, a useful exploration calculations can be carried out using the constant density model, since the generated axial velocity component is very small,  $0.0 \leq |u| \leq 0.04$  and also the variation in  $v$  is consistent with the mass conservation. In general, the Navier-Stokes model, it is our believe, may have a significant effect when the current solution to the modeling of randomly packed heterogeneous propellant, particularly in 3-D solution is advanced.

## 5. CONCLUSION

Here, for the first time, the 2D calculations to the combustion of heterogeneous solid propellant, accounting for the gas phase physics, the solid phase physics and an unsteady non-planar description of the regressing propellant surface is developed. There are a number of issues that have discussed. The speed within which the combustion surface recedes depends on the exposed pressure in the gas phase, the effect of several parameters on the combustion and

shape of the flame. In addition a variety of steady-state surface shapes are achieved. At higher pressure values, the binder is tend to stick out and the surface consists of a "trough" centered on the binder lamina. These trends were also recognized in an experimental observation [5].

A comparison between the computational steadily surface regressing profile with the experimental emission-transmission composite image by Brewster, et al. (2001), [26] and also with the experimental photography for the spontaneous quench samples of AP/BPAN/AP sandwich that reported by Lee et al. [4] is qualitatively consistent.

In this study, the Navier-Stokes equations were used rather the constant density model in earlier work [7,10,16, and 18]. A comparison between the constant density model and the Navier-Stokes solutions reveals very small differences. As a results, the Navier-Stokes model may have a significant effect when our solution to the modeling of randomly packed heterogeneous propellant, particularly in 3-D solution is advanced.

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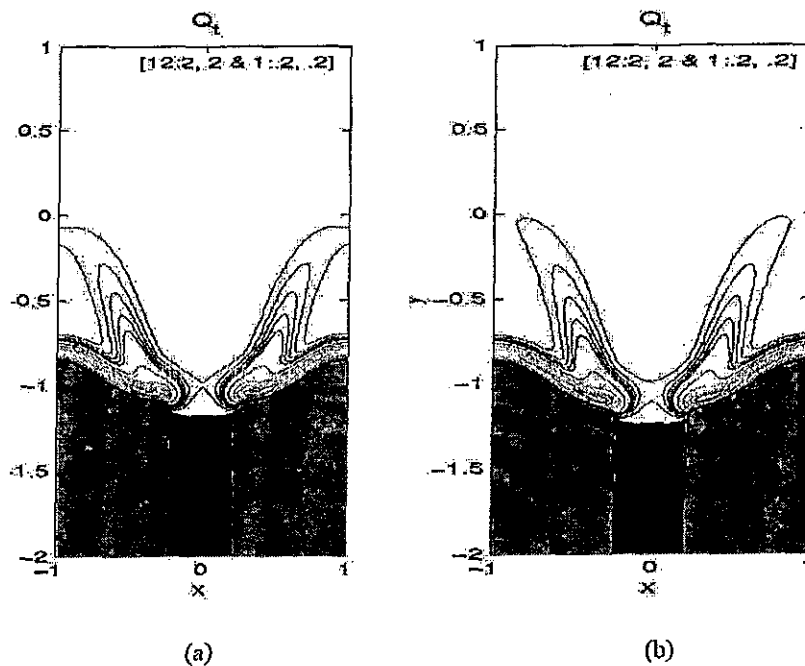


Fig. (8): Total reaction rate contours (a) Constant density model, (b) Variable density model

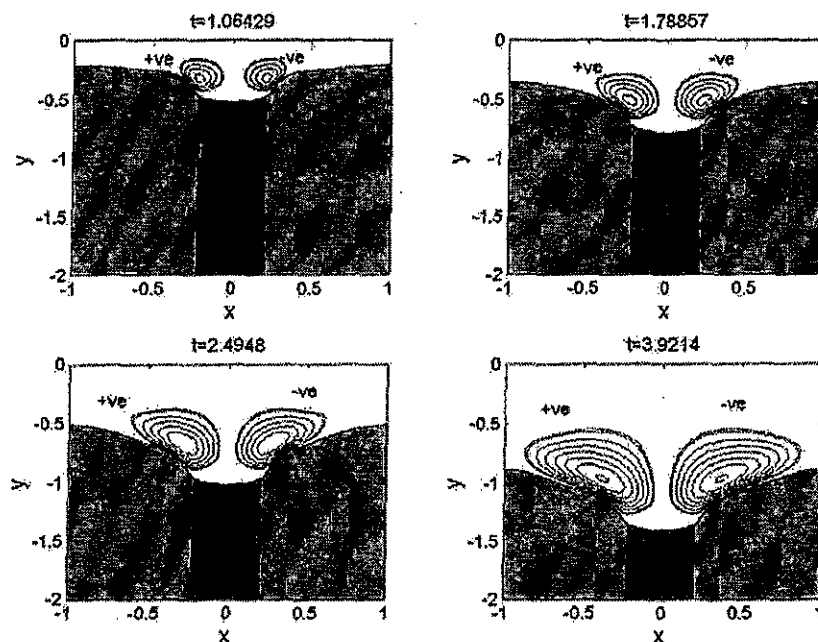


Fig. 9. The axial velocity component for the variable density model (2) at different times for  $M=0.02$ .

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