

# MULTIPLE INTEGRAL-BALANCE METHOD:

## Basic idea and an example with Mullin's model of thermal grooving

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### Abstract

*A multiple integration technique of the integral-balance method allowing solving high-order diffusion equations is conceived in this note. The new method termed multiple-integral balance method (MIM) is based on multiple integration procedures with respect to the space coordinate and is generalization of the widely applied Heat-balance integral method of Goodman and the double integration method of Volkov. The method is demonstrated by a solution of the linear diffusion models of Mullins for thermal grooving*

**Keywords:** Multiple-integration method, high-order no-linear diffusion, Mullins equation

### 1. INTRODUCTION

The integral-balance method [1,2] to diffusion models of heat and mass employs a concept of a penetration depth thus defining a sharp front of propagation. Integral-balance solutions are extensively used [3,4] and still attractive for solutions of non-linear diffusion problems [4-8]. This communication conceives the idea of the **Multiple-Integral Method (MIM)** which can be considered as a generalization of the integral-balance approach beyond the Heat-Balance Integral of Goodman [1] and the Double-Integration Method of Volkov [9].

### 2. The integral-balance method: Existing background as integration techniques

#### 2.1. The classical approach: basic concept

Transient diffusion (heat or mass) in a homogeneous medium with a constant transport coefficient (diffusivity)  $a$  is modelled by the parabolic equation in dimensionless form (with respect to the temperature (concentration) only)

$$\frac{\partial \theta}{\partial t} = a \frac{\partial^2 \theta}{\partial x^2}, \quad \theta(x, t) = 0 \quad \text{for } t > 0 \quad (1)$$

In the case of a semi-infinite medium the value of  $\theta(x, t)$ , far away from the boundary  $x=0$ , is assumed  $\theta(\infty, t) = 0$ . The sharp front concept replaces these conditions by new ones  $\theta(\delta, t) = \partial \theta(\delta, t) / \partial x = 0$ .

The simplest method known as *Heat-balance Integral Method (HBIM)* [1,2] suggests integration of eq. (1) with respect to the space co-ordinate over a finite penetration depth  $\delta$ , namely

$$\frac{d}{dt} \int_0^{\delta} \theta(x, t) dx - \theta(\delta, t) \frac{d\delta}{dt} = \int_0^{\delta} a \frac{\partial^2 \theta}{\partial x^2} dx \Rightarrow \frac{d}{dt} \int_0^{\delta} \theta(x, t) dx = -a \frac{\partial \theta}{\partial x}(0, t) \quad (2a, b)$$

Replacing  $\theta$  by an approximate profile  $\theta_a$ , an ordinary differential equation describing the time-evolution of  $\delta(t)$  can be derived. The principle problem of HBIM is the approximation of the gradient of right-side of (3b) *because it should be defined through the assumed profile*.

The *Double-Integration Method (DIM)* [6,7,9] in its classical formulation uses two steps: integration with respect to the space coordinate from 0 to  $x$  and a second step as integration from 0 to  $\delta$  (see eq.3a). Here will use a more general definition of DIM (see eq.3b) developed in [7] allowing application to cases with integer-order [6] (as in the present case) and time-fractional derivatives [7]. With a consequent application of the Leibniz rule we have the following expressions

$$\frac{d}{dt} \int_0^{\delta} \left( \int_0^x x \theta(x,t) dx \right) dx = a_0 \theta(0,t) \quad \text{or} \quad \frac{d}{dt} \int_0^{\delta} \left( \int_x^{\delta} \theta(x,t) dx \right) dx = a_0 \theta(0,t) \quad (3a,b)$$

## 2.2. Boundary characteristic approach

Recently the *Method of Boundary Characteristics (MBC)* as an improvement of the integral-balance method was proposed by Kot [10] for solution of the model (1). The principle steps of MBC suggest application of a sequence of integral operators (4a) in the interval  $[x, \delta(t)]$  and over a finite interval  $[0, \delta(t)]$  (4b), namely

$$L_n^x = \overbrace{\int_{\delta(t)}^x \int_{\delta(t)}^x (\dots) dx^2 \dots \int_{\delta(t)}^x \int_{\delta(t)}^x (\dots) dx^2}^n, \quad L_n = \overbrace{\int_{\delta(t)}^0 \int_{\delta(t)}^x (\dots) dx^2 \dots \int_{\delta(t)}^0 \int_{\delta(t)}^x (\dots) dx^2}^n \quad (4a,b)$$

The technology of MBC requires additional boundary conditions at  $x=0$  and polynomial assumed profiles up to the 8th order. The principle step of MBC is that after application of  $L_n^x$  the coordinate  $x$  is set to  $x=0$ . At this point we stop to comment MBC because it is beyond the scope of the present work but it was commented only to show its idea and to make clear the existing background thus allowing demonstrating the basic principle MIM and its differences with respect to MBC; as well as avoiding any misunderstandings in interpretation of the proposed generalization of the integration technique.

## 3. Multiple-integration method (MIM): Definitions

To present the basic idea of the method let us consider a diffusion equation of order  $p$

$$\frac{\partial \theta}{\partial t} = b \frac{\partial^p \theta}{\partial x^p}, \quad b > 0, \quad p \geq 2 \quad (5)$$

### 3.1. Definition of the multiple integral operators $L_k$

The multiple-integration method suggests applying the operator  $L_k$ , on a diffusion equation of order  $p$  defined as ( and applying the Leibnitz rule- see eq.2 and eq.3)

$$\frac{d}{dt} \underbrace{\int_0^{\delta} \left\{ \underbrace{\int_x^{\delta} \int_x^{\delta} \int_x^{\delta} \theta(x,t) dx dx dx}_{k-1} \right\}}_k dx = \int_0^{\delta} \underbrace{\left\{ \underbrace{\int_x^{\delta} \int_x^{\delta} \int_x^{\delta} \left[ b \frac{\partial^p}{\partial x^p} \theta(x,t) \right] dx dx dx}_{k-1} \right\}}_k dx \quad (6)$$

Therefore, we have to perform  $k-1$  integrations from  $x$  to  $\delta$  and the last  $k^{th}$  integration should be from 0 to  $\delta$ . Now, applying  $L_k$  to the model (1), by help of the Leibnitz rule, we get (6).

The number of integrations that should be applied in (6) depends on the order of the diffusion term  $p$  and the general rule is  $k = p$ . However, when  $k \leq p$  is applied we get

$$\underbrace{\int_0^\delta \left\{ \int_x^\delta \int_x^\delta \int_x^\delta \left[ b \frac{\partial^p}{\partial x^p} \theta(x,t) \right] dx dx dx \right\} dx}_k = b \frac{\partial^{p-k}}{\partial x^{p-k}} \theta(0,t) \quad (7)$$

In accordance with (7), if  $k = 1$  and  $p = 2$ , we get the integral relation of the HBIM expressed by (2a,b). Further, for  $k = p = 2$  we actually apply DIM expressed by (3a,b).

## 4. MIM to the Mullins equation of thermal grooving

### 4.1. Mullins diffusion model

In processes of groove growths by mechanism of evaporation-condensation the surface profile satisfy the non-linear diffusion equation (with boundary and initial conditions) [11,12]

$$\frac{\partial u}{\partial t} = \left[ \frac{D(0)}{1 + (\partial u / \partial x)^2} \right] \frac{\partial^4 u}{\partial x^4}, \quad \frac{\partial u(0,t)}{\partial x} = u_0 = const., \quad \frac{\partial u(x,t)}{\partial x} \rightarrow 0 \text{ as } x \rightarrow \infty, \quad u(x,0) = 0 \quad (8a,b,c)$$

With the assumption of symmetric groove shape about  $x = 0$ , the problem could be considered only along the half-line  $x \geq 0$  (see Fig.1a). The nonlinear model (1) has been solved exactly by Broadbridge [12,13] and other authors [14,15] but the solutions are hard to be physically analyzed. In case of a small curvature of the surface and the assumption that the evaporation is the sole mass transfer mechanism it is possible to linearize (8a) as

$$\frac{\partial u}{\partial t} = -B \frac{\partial^4 u}{\partial x^4}, \quad \frac{\partial u(0,t)}{\partial x} = m, \quad m > 0, \quad \frac{\partial^3 u(0,t)}{\partial x^3} = 0 \quad (9a,b,c)$$

In eq.(9b) the diffusion coefficient is  $B = D_s \gamma \Omega^2 \nu / kT$ , where:  $D_s$  is the coefficient of surface diffusion;  $\gamma$  is the free surface energy per unit area;  $\Omega$  is the molecular volume;  $\nu$  is the area where the diffusion takes place. The condition (9c) at  $x = 0$  corresponds to the requirement the flux to equals to zero at the origin [10,14]. Equation (9a) will be used to demonstrate the solution technology of **MIM**.

### 4.2. MIM Solution

To be the solution more familiar to known problems in transient diffusion we invert the *profile of the groove* from the original one with a *positive curvature* (see fig. 1b) to a *mirror profile* with a *negative curvature* (see fig.1a). The inverted groove profile mimics the decaying temperature (concentration) distribution with a typical Neumann problem, where the boundary condition is  $u_x(0,t) = -m$  (the sign in eq.(9b) changes since the curvature of the inverted profile is negative). Consequently the diffusion coefficient in eq.(9a) changes from  $-B$  to  $B$  and the equation becomes as the one presented by eq. (5) with  $p = 4$ .

The integral method, in general, requires the assumed profile to satisfy the conditions at both ends of the diffusional penetration depth. The assumed profile with unspecified exponent [3,4,5,6,7] is defined as  $u_a = u_s (1 - x/\delta)^n$  and used to demonstrate the technology of **MIM**. Its principle advantage is that *there*

is a freedom to optimize the accuracy of approximation by the mean squared error of approximation of the governing equation [4,6,7,11].

Next, applying the boundary condition (9b) we may define  $u_s = u_a(0,t) = m(\delta/n)$  as in the classical Neumann problem solved by HBIM and DIM [3,4]. In this notation,  $u_s = d + h$  is the groove depth, while  $\delta$  equals the half width of the groove ( $\delta = w/2$ ) from the symmetry axis to the inflection point (see Fig.1a and 1b) where the following conditions  $u_x(\delta) = u_{xx}(\delta) = u_{xxx}(\delta) = 0$  are valid.

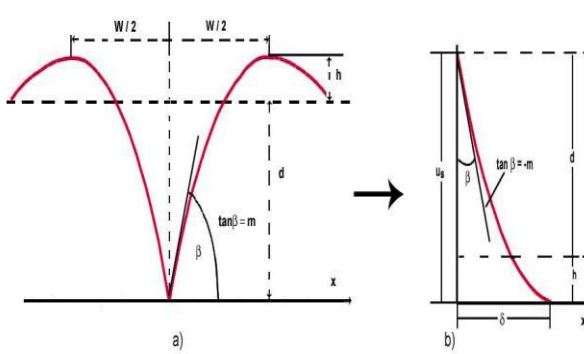


Fig.1. Sketch of the groove real profile (a) and the inverted (mirror) profile (b) used in the MIM solution

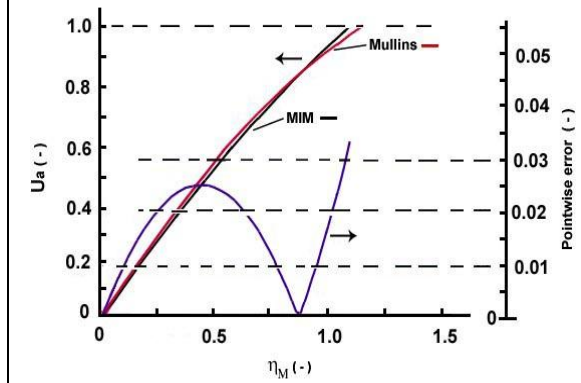


Fig.2. Approximate solutions : By Mullins and MIM, and the pointwise errors

Now, denoting  $z = x/\delta$  that transforms the moving boundaries  $0 \leq x \leq \delta$  to fixed Zener's coordinates  $0 \leq z \leq 1$ , and changing the variables in the integrals in the left-hand side of eq.(6) we have for  $k = 4$  (defined by the order of derivative in the right-hand side of eq.8a)

$$\frac{d}{dt} \int_0^1 \delta^5 \left( \frac{m}{n} \right) \left\{ \int_z^1 \int_z^1 \int_z^1 [z(1-z)^n] dz dz dz \right\} dz = mBu(0,t) \Rightarrow \frac{d}{dt} \delta^5 = B\delta \frac{N_4}{n} \quad (10ab)$$

$$N_4 = n(n+1)(n+2)(n+3)(n+4) = n! = \Gamma(n+k) \quad , \quad k = 4$$

The solution of eq.(10b) with the initial condition  $\delta(t=0) = 0$  is  $\delta = (Bt)^{1/4} M_4^{1/4}$ , where  $M_4 = (5/4)(\Gamma(n+4)/n)$ . Therefore, the groove surface profile can be approximated by

$$u_a(x,t) = \frac{m}{n} (Bt)^{1/4} M_4^{1/4} \left( 1 - \frac{x}{(Bt)^{1/4} M_4^{1/4}} \right)^n \Rightarrow U_a = \frac{u_a}{m(Bt)^{1/4}} = \frac{M_4^{1/4}}{n} \left( 1 - \frac{x}{(Bt)^{1/4} M_4^{1/4}} \right)^n \quad (11a,b)$$

The normalized profile  $U_a$  is presented in a way similar to that used by Mullins [11] (see eq. 12) and mimics the solution of the classical Newman problem when  $p = 2$ . For  $x = 0$  we get the temporal growth of the groove depth which in the original configuration (see fig. 2) should be  $u_s = -(m/n)(Bt)^{1/4} M_4^{1/4}$ .

The mean squared displacement  $\langle x^2 \rangle$  of the diffusion process is defined as  $\langle x^2 \rangle = \int_0^\infty xu(x,t)dx$ . With the assumed profile  $u_a$  and upper terminal of the integral fixed at  $\delta$  we have  $\langle x^2 \rangle \equiv \delta^2$  [14,15]. From the solution developed above it follows that  $\delta^2 \equiv t^{1/2}$  that immediately tells us that the surface diffusion process modelled by eq.(9) is subdiffusive in nature as it was analyzed in [16].

The approximate profile (11) defines in a natural way the non-Boltzmann similarity variable  $\eta_M = x/(Bt)^{1/4}$ . This similarly variable was used by Mullins [11] to transform eq.(10a) in an

ordinary differential equation. The solution of this transformed equation is analyzed by Robertson [14], but the main disadvantage is that the results are hard to be used for engineering applications and physical analyzes. Mullins [10] developed an approximate solution as a series of  $\eta_M$ , namely

$$u(x,t) = m(Bt)^{1/4} \sum_i^{\infty} a_i (\eta_M)^i \Rightarrow U(x,t) = \sum_i^{\infty} a_i (\eta_M)^i, U(x,t) = u(x,t) / \left[ m(Bt)^{1/4} \right] \quad (12)$$

The solution was carried out over the range from  $m=0$  to  $m=4$  accepting in all cases  $(Bt)^{1/4} = 1$  (**sic!**) and expressing the profile with respect to the spatial coordinate  $x$  and 16 terms of the series (12) (see Table 1 in [11]).

The exponent  $n$  of the approximate solution (11a,b) can be easily determined by the least-squared method minimizing the residual function of eq.(9) when  $u(x,t)$  is replaced by  $u_a$ . That is  $R = (u_a)_t - B(u_a)_{xxx}$  has to be minimized with respect to  $n$ , which means application of the Langford method for integral-balance solutions [2]. Details of this optimization procedure, commonly applied in integral-balance solutions since 2009 [3,4,6] are available elsewhere [3,4,5,6,7].

Since the parameter  $m$  is a pre-factor of the profile but it does not affect  $\delta$ , then the minimization of the residual function  $R$  is independent of  $m$ . In this context, it is noteworthy, that the validity of the solution when  $x \rightarrow \delta$  imposes the requirement  $n > 4$ , similar to the case with  $p=2$  (see eq.1) where the requirement is  $n > 2$  [6,7]. The present study established an optimal exponent  $n_{opt} \approx 4.55$ . The approximate solutions by MIM (eq.11) and that of Mullins (eq.12) are presented at Fig. 2. It clear that the MIM solution errors of approximation fall into the common range of  $2 \div 3\%$  [6,7]. Moreover, MIM as an integral-balance method with a finite penetration depth works only within the range  $0 \leq x \leq \delta$  or equivalently when  $0 \leq \eta_M \leq \left[ (Bt)M_4 \right]^{1/4}$ .

## Conclusions

This note conceives a novel integral-balance method (solution technique) named Multiple-Integral Method (**MIM**) which a generalization of the existing Heat-balance integral of Goodman and the Double integration method of Volkov. The method allows solving diffusion equations of high order and the solution example with the Mullins equation of thermal groove growing is a good demonstration of its feasibility to solve equation beyond the classical diffusion models.

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