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On the convergence of the heat balance integral method

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Abstract

Convergence properties are established for the piecewise linear heat balance integral solution of a benchmark moving boundary problem, thus generalising earlier results [Numer. Heat Transfer 8 (1985) 373]. A convergence rate of $O(n^{-1})$ is identified with minor effects at large values of the Stefan number β (slow interface movement). The correct $O(n^{-1/2})$ behaviour for incident heat flux is recovered for $\beta \to 0$ (pure heat conduction) as previously found [Numer. Heat Transfer 8 (1985) 373–382]. Numerical illustrations support the theoretical findings.
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1. Introduction

Goodman's heat balance integral (HBI) method [1] is one of many semi-analytical techniques [2] that may be used to generate functional approximations to transport problems governed by differential equations. Spatial boundary conditions are satisfied by the selected approximant, together with an integral form of the governing equation. Goodman constructed quadratic temperature profiles for transient one-dimensional heat transfer both with and without phase change,

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although it should be noted that the original interpretation of the intrinsic boundary conditions can be improved upon [3].

Since Goodman's original work [1] several proposals have improved the accuracy of the basic method. Here we focus upon spatial and temperature sub-division coupled with low-order piecewise approximants that circumvent the usual sensitivity of the HBI to the selected approximant and which 'flavoured' research papers from the mid 1970s.

Noble [4] suggested the combination of spatial sub-division and low-order piecewise approximants as a refinement of the HBI method. Bell [5,6] demonstrated the effectiveness of the approach using piecewise linear approximants and only a few sub-divisions for problems in plane and radial geometries. Bell [7] introduced temperature sub-division and the modification was successfully applied to the two-phase solidification problem of estimating the penetration depth of frost [8]. In these papers numerical evidence of convergence is presented, and in 1985 Bell and Abbas [9] formally established the convergence of a piecewise linear HBI solution to the problem of pure heat conduction in a semi-infinite medium.

The present work generalises the formal convergence analysis to the set of one-phase melting problems that is often cited for 'test purposes' of which the problem addressed by Bell and Abbas [9] is a special limiting case.

2. A model problem

The analysis presented in this paper is based upon a dimensionless mathematical description of the single-phase melting of ice [10],

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2}, \quad 0 < x < s(t), \quad t > 0, \tag{1}$$

$$U(0,t) = 1, \quad t > 0; \quad U(x,t) = 0, \quad x = s(t), \quad t > 0, \tag{2}$$

$$U(x,0) = 0, \quad x \geqslant 0, \tag{3}$$

$$\frac{\partial U}{\partial x} = -\beta \frac{\mathrm{d}s}{\mathrm{d}t}, \quad x = s(t), \quad t > 0. \tag{4}$$

Eq. (1) governs the flow of heat in the liquid region, Eq. (2) prescribes the temperature at the fixed boundary $x = 0$ and on the moving melt front $x = s(t)$, and Eq. (3) gives the initial temperature of the semi-infinite solution domain. The Stefan condition (4) describes the absorption of heat at the melt front [11] where the Stefan number $\beta = L/c(T_0 - T_m)$ is the ratio of latent to sensible heat. The analytical solution to Eqs. (1)–(4) is

$$U(x,t) = 1 - \frac{\operatorname{erf}(x/2\sqrt{t})}{\operatorname{erf}(\alpha)}, \quad 0 \leqslant x \leqslant s(t), \quad t \geqslant 0, \tag{5}$$

$$s(t) = 2\alpha\sqrt{t}, \quad t \geqslant 0, \tag{6}$$

where α is the root of the transcendental equation $\sqrt{\pi}\alpha\,\mathrm{erf}(\alpha)\mathrm{e}^{\alpha^2}\beta = 1$.

3. Piecewise linear HBI solution

To approximate the solution of the single-phase problem (1)–(4) the interval $[0, s]$ is sub-divided into n equal cells of length s/n and the temperature U is approximated at each node $x_i = is/n$ by $v_i \approx U(x_i, t)$ where $v_0 = 1$ and $v_n = 0$. A piecewise linear profile is chosen,

$$v = v_i + \frac{n(x - x_i)(v_{i+1} - v_i)}{s}, \quad x_i \leqslant x \leqslant x_{i+1}, \quad i = 0, \ldots, n-1, \tag{7}$$

having a piecewise-constant temperature gradient defined by

$$\frac{\partial v}{\partial x} = \frac{n(v_{i+1} - v_i)}{s}, \quad x_i \leqslant x < x_{i+1}, \quad i = 0, \ldots, n-1, \tag{8}$$

$$\frac{\partial v}{\partial x} = -\beta\frac{\mathrm{d}s}{\mathrm{d}t}, \quad x = s(t). \tag{9}$$

On each cell U is replaced by v and a heat balance integral is constructed from Eq. (1) of the form

$$\int_{x_i}^{x_{i+1}} \frac{\partial v}{\partial t}\,\mathrm{d}x = \left.\frac{\partial v}{\partial x}\right|_{x=x_{i+1}} - \left.\frac{\partial v}{\partial x}\right|_{x=x_i}, \quad i = 0, \ldots, n-1. \tag{10}$$

Combining Eqs. (7)–(10) generates n ordinary differential equations

$$s\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{2n^2}{2i+1}\,\frac{v_{i+2} - 2v_{i+1} + v_i}{v_i - v_{i+1}}, \quad i = 0, \ldots, n-2, \tag{11}$$

$$s\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{2n^2 v_{n-1}}{(2n-1)v_{n-1} + 2n\beta}. \tag{12}$$

On equating Eqs. (11) and (12), a system of $n-1$ non-linear equations in terms of the $n-1$ unknown temperatures $v_1, \ldots, v_{n-1}$ is produced of the form

$$v_i = v_{i+1} - f_i(v_{i+2} - v_{i+1}), \quad i = n-2, n-3, \ldots, 0, \tag{13}$$

where

$$f_i = \frac{n + \eta - 1/2}{n + \eta - i - 1}, \quad \eta = \frac{n\beta}{v_{n-1}}. \tag{14}$$

With $i = n-2$ and $i = n-3$ in Eq. (13),

$$\begin{aligned}
v_{n-2} &= v_{n-1}(1 + f_{n-2}),\\
v_{n-3} &= v_{n-2} - f_{n-3}(v_{n-1} - v_{n-2})\\
&= v_{n-1}(1 + f_{n-2} + f_{n-2}f_{n-3}),
\end{aligned}$$

and continuing the back substitution it is not difficult to show that v_i can be expressed as

$$v_i = v_{n-1}\left[1+\sum_{\ell=i}^{n-2}\prod_{j=\ell}^{n-2} f_j\right] = v_{n-1}\sum_{\ell=i}^{n-1}\frac{(n+\eta-1/2)^{n-\ell-1}}{(n+\eta-\ell-1)!}\eta! = v_{n-1}\sum_{k=0}^{n-i-1}\frac{(n+\eta-1/2)^k}{(\eta+k)!}\eta! \tag{15}$$

Enforcing the condition $v_0 = 1$,

$$v_{n-1}\sum_{k=0}^{n-1}\frac{(n+\eta-1/2)^k}{(\eta+k)!}\eta! = 1, \tag{16}$$

and eliminating v_{n-1} between Eqs. (15) and (16) yields

$$v_i = \frac{\sum_{k=0}^{n-i-1}\frac{(n+\eta-1/2)^k}{(\eta+k)!}}{\sum_{k=0}^{n-1}\frac{(n+\eta-1/2)^k}{(\eta+k)!}}, \quad i = 0,\ldots,n-1. \tag{17}$$

At this point we note that the formula obtained by Bell and Abbas [9] for a semi-infinite pure heat conduction problem was (in the present notation)

$$v_i = \frac{\sum_{k=0}^{n-i-1}\frac{(n-1/2)^k}{k!}}{\sum_{k=0}^{n-1}\frac{(n-1/2)^k}{k!}}, \quad i = 0,\ldots,n-1.$$

The present work introduces η (to give Eq. (17)) which is a non-linear function of n that captures the effect of the melt front s moving with a finite speed. For pure heat conduction [9] $\beta = 0$ and $\eta = 0$ (see Eq. (14)).

For $\beta > 0$ and $n > 0$, η is obtained from a non-linear equation generated by Eq. (16) on replacing v_{n-1} by $n\beta/\eta$ (see Eq. (14)). Once η is determined the v_i are found from Eq. (17) and s is estimated from the solution of Eq. (12),

$$s = \frac{2n\sqrt{t}}{\sqrt{2n+2\eta-1}} = 2\alpha^*\sqrt{t}, \quad \alpha^* = \frac{n}{\sqrt{2n+2\eta-1}}. \tag{18}$$

α^* is to be interpreted as an approximation to the melt parameter α. For $\beta = 1$ and $n = 10$, 20 and 40 intervals, Table 1 lists values of α^*, the mid-domain temperature $v(s/2,1)$ and the incident heat flux $v'(0,1)$ from

Table 1
Estimates of the melt parameter, the mid-domain temperature and the incident heat flux (piecewise linear HBI with $\beta = 1$ and n intervals)

n	α^*	$v(s/2,1)$	$v'(0,1)$
10	0.6139	0.4575	−0.9038
20	0.6170	0.4552	−0.9072
40	0.6185	0.4540	−0.9090
Exact	0.6201	0.4528	−0.9108

$$\frac{\partial v}{\partial x} = \frac{n(v_1 - 1)}{s}. \tag{19}$$

It is clear that the selected parameters converge to the analytical values and extrapolation identifies numerical convergence rates of 0.97, 1.01 and 0.94, respectively.

4. Analysis of convergence

In formally establishing the convergent behaviour observed in Table 1, the analysis naturally includes the entire range of physical problems described by the model (1)–(4), from pure heat conduction ($\beta \to 0$) to slow phase change ($\beta \to \infty$). It will be seen that the convergence of the numerical method depends upon β and to illustrate the methodology, the behaviour of the incident heat flux (19), is considered in the limit $n \to \infty$.

Combining Eqs. (17)–(19) gives the approximate incident heat flux

$$\left.\frac{\partial v}{\partial x}\right|_{x=0} = -\frac{(n+\eta-1/2)^{n-1/2}}{\sqrt{2t}(n+\eta-1)!\sum_{k=0}^{n-1}\frac{(n+\eta-1/2)^k}{(\eta+k)!}}. \tag{20}$$

Defining

$$\Phi(m,\eta,z) = \sum_{k=0}^{m-1}\frac{z^k}{(\eta+k)!}, \quad I(m) = \frac{(m-1/2)^{m-1/2}}{\Gamma(m)\mathrm{e}^{m-1/2}}, \tag{21}$$

and [12, Eq. 6.5.22] using the identity $\gamma(a,z) = (a-1)\gamma(a-1,z) - e^{-z}z^{a-1}$ (m times), where the incomplete gamma function γ is defined by [12, Eq. 6.5.2]

$$\gamma(a,z) = \int_0^z \mathrm{e}^{-t}t^{a-1}\,\mathrm{d}t,$$

it is a fairly straightforward matter to show that

$$\Phi(m,\eta,z) = \mathrm{e}^z z^{-\eta}\left[\frac{\gamma(\eta,z)}{\Gamma(\eta)} - \frac{\gamma(m+\eta,z)}{\Gamma(m+\eta)}\right]. \tag{22}$$

Eq. (20) may then be written

$$\left.\frac{\partial v}{\partial x}\right|_{x=0} = -\frac{I(n+\eta)}{\sqrt{2t}\left[\frac{\gamma(\eta,n+\eta-1/2)}{\Gamma(\eta)} - \frac{\gamma(n+\eta,n+\eta-1/2)}{\Gamma(n+\eta)}\right]}. \tag{23}$$

To examine the behaviour of Eq. (23) as $n \to \infty$, several results are required.

- For large m [9]

$$I(m) = \frac{1}{\sqrt{2\pi}}\left[1 + \frac{1}{24m} + \cdots\right] = \frac{1}{\sqrt{2\pi}}[1 + \mathrm{O}(m^{-1})]. \tag{24}$$

- Combining Pearson's formula [13]

$$\gamma(m+1,z) = e^{-m}m^{m+1/2}\sqrt{\frac{\pi}{2}}\left[1+\operatorname{erf}\left(\frac{z-m}{\sqrt{2m}}\right)+O(m^{-1/2})\right],$$

where m is large and $0 < z < 2m$, and Stirling's formula [12, Eq. 6.1.37]

$$\Gamma(m) \sim e^{-m}m^{m-1/2}\sqrt{2\pi}\left[1+\frac{1}{12m}+\frac{1}{288m^2}+\cdots\right], \quad m\to\infty,$$

with the familiar result

$$\lim_{m\to\infty}\left(1-\frac{1}{m}\right)^{m-1/2} = e^{-1},$$

we obtain (for large m) the limiting form

$$\frac{\gamma(m,z)}{\Gamma(m)} = \frac{1}{2}\left[1+\operatorname{erf}\left(\frac{z-m}{\sqrt{2m}}\right)+O(m^{-1/2})\right]. \tag{25}$$

Using formula (24) with $m = n + \eta$ and formula (25) with (i) $m = \eta$ and $z = n + \eta - 1/2$ and (ii) $m = n + \eta$ and $z = n + \eta - 1/2$, the 'large n' behaviour of the terms appearing in Eq. (23) can be expressed as

$$I(n+\eta) = \frac{1}{\sqrt{2\pi}}\left[1+O\left(\frac{1}{n+\eta}\right)\right], \tag{26}$$

$$\frac{\gamma(n+\eta,n+\eta-1/2)}{\Gamma(n+\eta)} = \frac{1}{2}\left[1+O\left(\frac{1}{\sqrt{n+\eta}}\right)\right], \tag{27}$$

$$\frac{\gamma(\eta,n+\eta-1/2)}{\Gamma(\eta)} = \frac{1}{2}\left[1+\operatorname{erf}\left(\frac{n}{\sqrt{2\eta}}\right)+O\left(\frac{1}{\sqrt{\eta}}\right)\right]. \tag{28}$$

To simplify the last result we note from Eq. (14) that

$$\eta = \frac{n\beta}{v_{n-1}} = n\beta\eta!\sum_{k=0}^{n-1}\frac{(n+\eta-1/2)^k}{(\eta+k)!}.$$

The kth term is bounded below by 1 if $n \geqslant k+1$, which must hold for each term in the summation. That is

$$\eta!\frac{(n+\eta-1/2)^k}{(\eta+k)!} \geqslant 1, \quad k = 0,\ldots,n-1,$$

and hence

$$\eta!\sum_{k=0}^{n-1}\frac{(n+\eta-1/2)^k}{(\eta+k)!}\geqslant n.$$

Consequently, $\eta>\beta n^2$ and for large n

$$\alpha^*=\frac{n}{\sqrt{2n+2\eta-1}}\sim\frac{n}{\sqrt{2\eta}}. \tag{29}$$

For fixed s and large n

$$\alpha=\frac{s}{2\sqrt{t}}\simeq\alpha^*\to\frac{n}{\sqrt{2\eta}}\Rightarrow n\to\sqrt{2\eta}\alpha \tag{30}$$

and Eq. (28) behaves as

$$\frac{\gamma(\eta,n+\eta-1/2)}{\Gamma(\eta)}=\frac{1}{2}\left[1+\mathrm{erf}(\alpha)+\mathrm{O}\left(\frac{1}{\sqrt{\eta}}\right)\right]. \tag{31}$$

Collecting together the limiting forms (26), (27) and (31), the behaviour of Eq. (23) can be expressed as

$$\left.\frac{\partial v}{\partial x}\right|_{x=0}=-\frac{\frac{1}{\sqrt{2\pi}}\left[1+\mathrm{O}\left(\frac{1}{n+\eta}\right)\right]}{\sqrt{2t}\left\{\frac{1}{2}\left[1+\mathrm{erf}(\alpha)+\mathrm{O}\left(\frac{1}{\sqrt{\eta}}\right)\right]-\frac{1}{2}\left[1+\mathrm{O}\left(\frac{1}{\sqrt{n+\eta}}\right)\right]\right\}}.$$

In other words,

$$\left.\frac{\partial v}{\partial x}\right|_{x=0}\to-\frac{1}{\sqrt{\pi t}\,\mathrm{erf}(\alpha)},\quad n\to\infty \tag{32}$$

and the numerical estimates of the incident heat flux formally converge to the exact value. A little algebra shows the rate of convergence to be proportional to $(n+\eta)^{-1/2}$, i.e. $(n+\beta n^2)^{-1/2}$. For $\beta>0$ (including typical phase change, $\beta\simeq 1$, and slower processes, large β) the term βn^2 dominates and the asymptotic rate is $\mathrm{O}(n^{-1})$. If $\beta=0$ (pure heat conduction) the rate drops to $\mathrm{O}(n^{-1/2})$.

Similarly, we may consider the behaviour of the nodal temperature v_i as $n\to\infty$. Combining Eqs. (17), (21) and (22),

$$\begin{aligned}v_i&=\frac{\Phi(n-i,\eta,n+\eta-1/2)}{\Phi(n,\eta,n+\eta-1/2)},\quad i=0,\dots,n-1,\\&=\frac{\dfrac{\gamma(\eta,n+\eta-1/2)}{\Gamma(\eta)}-\dfrac{\gamma(n+\eta-i,n+\eta-1/2)}{\Gamma(n+\eta-i)}}{\dfrac{\gamma(\eta,n+\eta-1/2)}{\Gamma(\eta)}-\dfrac{\gamma(n+\eta,n+\eta-1/2)}{\Gamma(n+\eta)}}.\end{aligned} \tag{33}$$

The denominator and first term in the numerator have been considered (see Eqs. (27) and (31)) and attention is now focussed on a fixed point (x,t) where

$$\frac{is}{n} \leqslant x < \frac{(i+1)s}{n}.$$

Let $\xi = x/2\sqrt{t} = is/2n\sqrt{t}$, where $i \sim \xi\sqrt{2(n+\eta)}$ as $n \to \infty$. From Eq. (25)

$$\begin{aligned}\frac{\gamma(n+\eta-i, n+\eta-1/2)}{\Gamma(n+\eta-i)} &\simeq \frac{1}{2}\left[1+\operatorname{erf}\left(\frac{i-1/2}{\sqrt{2(n+\eta-i)}}\right)\right]\\ &= \frac{1}{2}\left[1+\operatorname{erf}(\xi)+\mathrm{O}\left(\frac{1}{\sqrt{n+\eta-i}}\right)\right]\end{aligned} \tag{34}$$

Eq. (33) therefore gives

$$\lim_{n\to\infty} v_i = 1 - \frac{\operatorname{erf}(x/2\sqrt{t})}{\operatorname{erf}(\alpha)} \tag{35}$$

for which convergence occurs at a rate proportional to $\eta^{-1/2}$, i.e. n^{-1}.

5. Numerical experiments

To provide evidence that theoretically established convergence rates obtained in Section 4 are observed in practice, we conclude with a few numerical experiments using the piecewise form of Section 3. The values $\beta = 10^{-2k}, k = 0, 1, 2$ are chosen to give evidence of behaviour as $\beta \to 0$ (pure heat conduction), shown in Table 2. Table 3 summarises results for large β (slow phase change).

From Table 2, for moderate values of β, the expected order of convergence is achieved, i.e. approximately linear. As β approaches zero (implying a latent heat of fusion tending to zero, and hence pure heat conduction) the order for the incident heat flux reduces to about 0.57 which is consistent with $\mathrm{O}(n^{-1/2})$ as indicated by the theory. The order for the mid-domain temperature $v(s/2,1)$ appears to increase. This can be explained. For small β the value $\eta \sim \beta n^2$ will not be dominant in the order terms for moderate values of n. In other words, for small β the expected asymptotic convergence behaviour will only become apparent for much larger values of n. In fact for the n-triple [8,16,32] the numerical order of convergence for $v(s/2,1)$ is 1.650 and for the triple

Table 2
Values of $\alpha^*, v(s/2,1)$ and $v'(0,1)$, together with convergence behaviour, as a function of small β

β		$n=10$	$n=20$	$n=40$	Exact	Order
0.0001	α^*	2.149412	2.442779	2.598143	2.760891	0.917
	v	0.102912	0.070857	0.059690	0.050820	1.521
	v'	−0.544193	−0.552218	−0.557623	−0.564243	0.570
0.01	α^*	1.665452	1.756491	1.803263	1.850946	0.961
	v	0.216905	0.198969	0.190899	0.183366	1.152
	v'	−0.553172	−0.560359	−0.564556	−0.569230	0.776
1.0	α^*	0.613937	0.616960	0.618502	0.620063	0.972
	v	0.457485	0.455156	0.453998	0.452845	1.009
	v'	−0.903820	−0.907202	−0.908965	−0.910777	0.941

Table 3
Values of $\alpha^*, v(s/2,1)$ and $v'(0,1)$, together with convergence behaviour, as a function of large β

β		$n=10$	$n=20$	$n=40$	Exact	Order
10	α^*	0.219756	0.219884	0.219950	0.220016	0.964
	v	0.494564	0.494262	0.494112	0.493962	1.001
	v'	−2.306655	−2.307946	−2.308610	−2.309286	0.960
100	α^*	0.070585	0.070589	0.070591	0.070593	0.963
	v	0.499439	0.499408	0.499393	0.499377	1.000
	v'	−7.093743	−7.094162	−7.094376	−7.094595	0.962
1000	α^*	0.022357	0.022357	0.022357	0.022357	0.963
	v	0.499944	0.499941	0.499939	0.499938	1.000
	v'	−22.367862	−22.367995	−22.368063	−22.368132	0.962

[16, 32, 64] the order is 1.319. This is consistent with the triple [10, 20, 40] appearing in Table 2 that gives an order of 1.521—the evidence suggests that the rate $O(n^{-1})$ is achieved for sufficiently large n.

Table 3 confirms the analysis for a range of increasing values of β, that convergence is linear, i.e. $O(n^{-1})$.

6. Conclusions

The analysis presented here has considered the convergence behaviour of a piecewise linear implementation of the heat balance integral method applied to a phase-change problem. The numerically observed rates of convergence have been rigorously established, and earlier 'special case' results [9] generalised. Of course, the analysis also highlights the rather slow convergence properties of the basic method (compared to the $O(n^{-2})$ expected of a standard finite-difference solver). An approach that uses a combination of mesh refinement and higher-order piecewise approximants for improving the convergence rate is currently being examined.

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