

# A GENERAL BOUNDARY-INTEGRAL FORMULATION FOR ZONED THREE-DIMENSIONAL MEDIA

*M. Rezaayat*

*Structural Dynamics Research Corporation  
Milford, Ohio, USA*

**Abstract** A new boundary-integral formulation is proposed to analyze the heat transfer in zoned three-dimensional geometries. The proposed formulation couples the boundary formula, the gradient of the boundary formula, and the exterior formula. An advantage of this formulation over the traditional methods is that any linear condition at the interface between subdomains may be incorporated into the formulation at the outset. In addition, the new method provides a sparse and well-conditioned matrix of coefficients with a minimum number of equations.

**Key Words** Boundary-Integral, Exterior formula, Three-Dimensional Media, Heat Transfer

**چکیده** یک فرمول بندی انتگرال مرزی جهت آنالیز انتقال حرارت در اجسام سه بعدی ارائه شده است. در این روش فرمولهای مرزی، مشتقات فرمولهای مرزی و فرمول بندی خارجی در هم ادغام شده اند. امتیاز روش ارائه شده در مقایسه با روشهای دیگر در این است که هرگونه شرایط خطی می تواند در مرز مشترک اجسام در شروع کار وارد عمل شود. بعلاوه، روش جدید یک ماتریس ضرایب با فضای خالی زیاد و خوش رفتار فراهم می کند که دارای حداقل تعداد معادلات می باشد.

## INTRODUCTION

The standard approach for solving zoned problems with the Boundary Element Method (BEM) is to write the integral equations for each zone, then couple the zones through additional compatibility and equilibrium conditions [1], thus, for perfect-contact interfaces (i.e., no resistance at the interface between zones), a problem with  $M$  nodes on the boundary and  $N$  nodes on the interfaces requires simultaneous solution of a system of  $M + 2N$  equations. Recently, an alternative method has been suggested [2, 3] which reduces the number of equations by introducing the compatibility and equilibrium conditions in the integral formulation at the outset. This direct approach leads to a system of  $M + N$  equations, and it can greatly reduce the operational cost during the formation of the matrix of coefficients. However, the matrix generated by this method is fully populated, whereas, through a judicious numbering scheme, the first method can

provide a banded matrix. On the other hand, only the latter method assures a well-conditioned matrix, since the former method places large coefficients off the diagonal. Both methods can only be applied to perfect contact problems; neither method is well suited to problems with a more general condition on the interface between subdomains.

A new formulation presented in this paper which generalizes the above methods while preserving the advantages of each. In this formulation, any linear condition at the interface between zones can be easily incorporated into the integral equations because the variables in the integral equations are written in terms of their sum and difference across the interface boundaries. The formulation couples the boundary formula, the gradient of the boundary formula, and the exterior formula. Combined with appropriate initial, boundary, and interface conditions, this combination forms a well-posed boundary-value problem and can be applied to problems with piecewise homogeneous domains. The resulting

coefficient matrix is fully populated since the formulation in effect couples the zones; however, an additional operation can improve this undesirable feature. In a previous publication [4], this author presented a method for reducing the bandwidth of BEM-generated matrices. That method, which is most effective when the whole domain is coupled, involves converting the fully populated system into a banded system by lumping certain coefficients of the matrix into fictitious nodes and then constraining these nodes to accurately represent each coefficient. The lumping procedure described in that paper is written for homogeneous domains; its extension to multidomain problems is straightforward and will be discussed here. Therefore, the proposed method, along with the application of lumping, provides a general formulation for heterogeneous problems with arbitrary conditions at the interfaces and leads to a banded, diagonally dominant matrix of coefficients with a minimum number of equations.

The motivation for this work is the need to analyze the steady-state thermal field in injection molds. Often, these molds contain blocks of dissimilar material for improved cooling. Also, blocks of movable metal may be used as a means of ejecting large parts from the mold. In this case the blocks of metal are similar, but the resistance at the interface between them has a marked effect on the cooling (in the area near the interface) and must be accounted for. Hence, the formulation must be general enough to apply to interfaces with and without gaps (i.e., with and without resistance to flow of heat at the interface) for similar as well as dissimilar materials. The formulation for each one of these cases is provided below.

### FORMULATION

Consider a three-dimensional region consisting of two subdomains (zones)  $V_1$  and  $V_2$  such that the first

subdomain is bounded by surfaces  $S_1$  and  $S_1^+$  and the second subdomain is bounded by surfaces  $S_2$  and  $S_1^-$ , as shown in Figure 1. (For simplicity, the derivation is given for two subdomains. The formulation will be extended to an arbitrary number of subdomains later in this section.) The conditions here are such that there is a resistance at the interface (represented in the form of a gap here); thus there is a discontinuity in temperature values on  $S_1^+$  and  $S_1^-$ . Now let a sufficiently smooth function  $T$  satisfy Laplace's equation within both  $V_1$  and  $V_2$ . Application of Green's second identity leads to the integral expressions [1]

$$\int_{\bar{S}_1} [K(P, Q) T_{,\mu}(Q) - K_{,\mu}(P, Q) T(Q)] dS(Q) = C_1(P) T(P) \quad (1)$$

and

$$\int_{\bar{S}_2} [K(P, Q) T_{,\mu}(Q) - K_{,\mu}(P, Q) T(Q)] dS(Q) = C_2(P) T(P) \quad (2)$$

where  $\bar{S}_1 = S_1 + S_1^+$ ,  $\bar{S}_2 = S_2 + S_1^-$ ,  $P$  and  $Q$  are two points in space (the so-called source and observation points),  $T$  is the temperature,  $T_{,\mu} = \partial T / \partial \mu$ ,  $\vec{\mu}$  is the outward unit normal at  $Q$ ,  $K$  is the fundamental solution to Laplace's equation -  $K = 1/4\pi |\vec{PQ}|^{-1}$

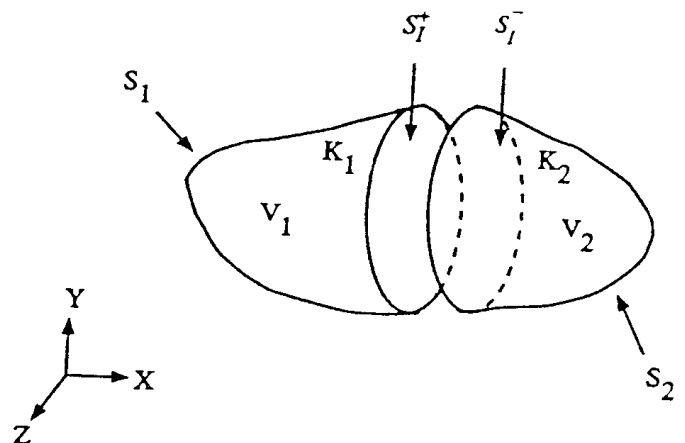


Figure 1. An example of multidomain geometry

$K_\mu = \partial K / \partial \mu$ , and

$$C_1(P) = \begin{cases} 1 & \text{for } P \in V_1 \Leftarrow \text{Interior formula} \\ 0 & \text{for } P \notin V_1 \Leftarrow \text{Exterior formula} \\ C_s & \text{for } P \in \bar{S}_2 \Leftarrow \text{Boundary formula} \end{cases} \quad (3)$$

and

$$C_2(P) = \begin{cases} 1 & \text{for } P \in V_2 \Leftarrow \text{Interior formula} \\ 0 & \text{for } P \notin V_2 \Leftarrow \text{Exterior formula} \\ C_s & \text{for } P \in \bar{S}_2 \Leftarrow \text{Boundary formula} \end{cases} \quad (4)$$

$C_s$  is proportional to the interior solid angle [5]. If  $\vec{\mu}$  is continuous at  $P$ , then  $C_s(P)$  is simply 1/2 everywhere on  $S_1$  and  $S_2$ . Now, multiply Equation 1 by  $k_1$ , the thermal conductivity for zone 1, and multiply Equation 2 by  $k_2$ , the thermal conductivity for zone 2. Add the two equations to get

$$\begin{aligned} & k_1 C_1(P) T_1(P) + k_2 C_2(P) T_2(P) = \\ & + \int_{S_1 + S_2} k [K(P, Q) T_\mu(Q) - K_\mu(P, Q) T(Q)] dS(Q) \\ & + \int_{S_1^+} k_1 [K(P, Q^+) T_\mu(Q^+) - K_\mu(P, Q^+) T(Q^+)] dS(Q) \\ & + \int_{S_2^-} k_2 [K(P, Q^-) T_\mu(Q^-) - K_\mu(P, Q^-) T(Q^-)] dS(Q) \end{aligned} \quad (5)$$

where, in the first integral,  $k$  and  $\mu$  take the proper subscript depending on the zone to which  $Q$  belongs. Given appropriate boundary and interface conditions, Equation 5, with 3 and 4, should provide a solution to this problem. However, because of the closeness of surfaces  $S_1^+$  and  $S_2^-$ , the form of this equation is inadequate for our problem [5]. The following sections present the necessary modifications to Equation 5.

### Case 1: Resistance at the Interface

If there is resistance to the flow of the heat across the interface itself, then the temperature is not continuous across the interface. However, it is valid to assume that the flux is continuous, and thus the compatibility conditions may be written as

$$k_1 T_\mu(Q^+) + k_2 T_\mu(Q^-) = 0 \quad (6)$$

where

$$T_\mu(Q^+) = -\frac{h}{k_1} [T(Q^+) - T(Q^-)] \quad (7)$$

One can, for instance, set  $h = k_a/b$  in which  $k_a$  is the thermal conductivity of air (assuming that the resistance is caused by a small air-filled gap) and  $b$  is the gap thickness.

Now, define the midsurface  $\Gamma$  with two faces such that the outward unit-normal vector at any point on one face (to represent  $S_1^+$ ) is opposite the outward unit-normal at its image on the opposite face (to represent  $S_2^-$ ). The new configuration is shown in Figure 2. Starting with the interior formula, first shrink the surfaces  $S_1^+$  and  $S_2^-$  onto  $\Gamma$ , then let  $P$  approach  $\Gamma$  from both sides [5]. After the limiting operation, the kernels in Equation 5 are related by

$$K(P, Q^+) = K(P, Q^-) \text{ and } K_\mu(P, Q^+) = -K_\mu(P, Q^-) \quad (8)$$

where  $Q^+$  and  $Q^-$  are images of one another on  $S_1^+$  and  $S_2^-$ , respectively. The negative sign leading  $K_\mu$  in

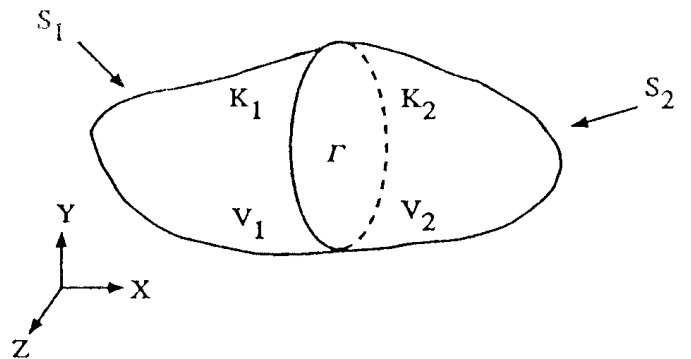


Figure 2. Midsurface  $\Gamma$  representing the interface

Equation 8 is caused by the opposing signs of  $\vec{\mu}$  on  $Q^+$  and  $Q^-$ . The sign convention adopted here is such that  $\vec{\mu}(Q^+) = \vec{\mu}(Q_\Gamma)$  and  $\vec{\mu}(Q^-) = -\vec{\mu}(Q_\Gamma)$ . Applying Equation 8 to Equation 5 after the limiting operation results in the following integral formula,

$$k_1 C_1(P) T_1(P) + k_2 C_2(P) T_2(P) = \int_S k [K(P, Q) T_\mu(Q) - K_\mu(P, Q) T(Q)] dS(Q) + \int_\Gamma [-K_\mu(P, Q^+) \Delta(kT(Q))] dS(Q) \quad (9)$$

where  $\Delta(kT) = k_1 T(Q^+) - k_2 T(Q^-)$ , and, as before,  $k$  in the first integral takes on the proper subscript according to the domain to which  $Q$  belongs. As shown in [5], the limiting operation from the other side results in an identical equation.

In Equations 9, 3, and 4 the difficulties associated with the integrations over closely-spaced surface have been removed. Unfortunately, these new formulae by themselves are not very useful because they cannot be combined with the usual set of boundary conditions to form a well-posed boundary-value problem [5]. To complete the set, an additional integral equation is required. The following procedure may be used to obtain this equation. First, take the gradient of the interior formula with respect to  $P$ . Next take the limit  $P \xrightarrow{(+)} \Gamma$  and perform the dot product with the unit normal to  $\Gamma$  at  $P$ . Finally, use the conditions at the interface defined above to obtain

$$-h [T(P^+) - T(P^-)] [C(P^+) + C(P^-)] = \int_S k [K_\nu(P, Q) T_\mu(Q) - K_{\mu\nu}(P, Q) T(Q)] dS(Q) + \int_\Gamma [-K_{\mu\nu}(P, Q^+) \Delta(kT(Q))] dS(Q) \quad (10)$$

where  $\nu$  is the outward unit normal at  $P$ ,  $K_\nu = \partial K / \partial \nu$ ,  $K_{\nu\mu} = \partial^2 K / \partial \nu \partial \mu$ , and once again  $k$  and  $\mu$  in the first integral take the proper subscript depending on the zone to which  $Q$  belongs. An additional simplification to this Equation is possible. Reference 6 shows that  $C(P^+) + C(P^-) = 1$ ; thus this term can be removed from Equation 10 without loss of generality.

With Equations 9, 3, 4, and 10, the interface between zones can now be efficiently modeled. The surfaces  $S$  and  $\Gamma$  are meshed using standard elements with the understanding that two degrees-of-freedom (DOFs) are associated with every node on  $\Gamma$ . Compared to the standard procedures, the numerical quadrature is a bit more involved here because of the existence of weakly singular, singular, and hypersingular integrands in Equations 9 and 10. One of several semi-analytical and numerical procedures may be used to reduce the order of the singularity [7, 8]. However, if piecewise-constant elements are used for discretization, as is the case here, a much simpler procedure may be used to obtain a closed-form integration of the singular integrands (see [5]).

The generalization of these equations for several zones is straightforward. For a set of  $M$  inserts, with a total of  $N$  interfaces, the following integral formula is used for all nodes

$$\sum_{i=1}^M k_i C_i(P) T_i(P) = \int_S k [K(P, Q) T_\mu(Q) - K_\mu(P, Q) T(Q)] dS(Q) + \sum_{j=1}^N \int_{\Gamma_j} -K_\mu(P, Q_j) [k_j T(Q_j) - k_{j'} T(Q_{j'})] dS(Q) \quad (11)$$

where  $\Gamma_j$  is the interface between subdomains  $j$  and  $j'$ , and  $k_j$  and  $k_{j'}$  are the corresponding thermal conductivities. For nodes on the interfaces, another integral formula is added to Equation 11 to complete the set. For instance, when  $P$  is one interface  $\Gamma_j$ , which is the

interface between zones  $l$  and  $l'$ , the additional integral equation is written as

$$-h[T_l(P)-T_{l'}(P)] = + \int_S k[K_\nu(P, Q)T_\mu(Q) - K_{\mu\nu}(P, Q)T(Q)] dS(Q) + \sum_{j=1}^N \int_{\Gamma_j} -K_{\mu\nu}(P, Q_j) [k_j T(Q_j) - k_{j'} T(Q_{j'})] dS(Q) \quad (12)$$

In both equations,  $S$  is the sum of all surfaces minus all the interfaces.

Note that even when the zones are all made of the same material, the thermal conductivity cannot be factored out from the last equation. This is because the thermal conductivity of the material affects the amount of discontinuity in temperature at the interface.

### Case 2: No Resistance at the Interface

The equations provided in the previous section can be used for simpler cases. For instance, when there is perfect contact at the interface between zones, compatibility and equilibrium conditions require that

$$T(Q^+) = T(Q^-) \text{ and } k_1 T_\mu(Q^+) + k_2 T_\mu(Q^-) = 0 \quad (13)$$

These conditions can be inserted into Equation 11 to get

$$\sum_{i=1}^M k_i C_i(P) T_i(P) = + \int_S k [K(P, Q) T_\mu(Q) - K_{\mu\nu}(P, Q) T(Q)] dS(Q) + \sum_{j=1}^N \int_{\Gamma_j} -K_{\mu\nu}(P, Q_j) (k_j - k_{j'}) T(Q) dS(Q) \quad (14)$$

which is sufficient for obtaining the temperature everywhere in the domain. (One cannot readily obtain the fluxes at the interface from Equation 14.

By differentiating the interior formula, however, it is possible to obtain an integral equation for temperature gradients across the interface.) Note that for the case where all subdomains are made of the same material, the thermal conductivity,  $k$ , can be removed, and this integral formula is reduced to the interior formula as expected. Also, normalizing the thermal conductivity in the above integral equations would make it possible to use the same formulation for zones made of the same material.

### BANDWIDTH REDUCTION

As stated before, the above formulation couples the zones leading to a system of equations with a fully populated matrix of coefficients. This is a serious drawback for large systems and must be addressed if the present method is to have widespread acceptability for analysis of realistic problems.

A novel approach to reduce the profile of matrices generated by the Boundary Element Method was presented in [4]. The method took advantage of the fact that the kernel functions in the integral formulas vary inversely with the distance between points in the domain, and thus certain contributions to the system's matrix are comparatively small and do not play an important role in the solution of the system. Reference 4 points out that these small contributions cannot be simply eliminated from the matrix because, although the coefficients are individually small, their combined effect cannot be ignored. The algorithm accounted for the combined effect of the small coefficients by creating fictitious nodes which represent the small coefficients in a lumped manner. Additional constraints defined the relationship between the real and fictitious unknowns. An efficient minimization algorithm was used to minimize the profile of the matrix, and an active column block-solver was used to solve the resulting system of equations. It was shown in [4] that the

algorithm can reduce the rate of increase of solution time  $t$  of an  $n$ -degree-of-freedom problem from  $t \propto n^3$  to  $t \propto n^2$ . The lumping method has been in use for several years [4], and its reliability and robustness have been demonstrated through the successful solution of many large matrices. That method can be easily extended to multidomain problems. The only major modification to the procedure described in [4] is inclusion of appropriate material properties in the identification process for lumping. In other words, the decision-making process for lumping a cluster of elements with respect to another cluster should include the effects of differing thermal conductivities. Normalizing the thermal conductivities in the integral equations can simplify the required modifications.

### APPLICATION

Recall that the new approach couples the boundary and the exterior integral formulas, which in turn couple the subdomains. In certain cases, this integral equation is by itself sufficient, while in other cases it has to be accompanied by its gradient. With this formulation, one can efficiently and accurately model the interface between similar and/or dissimilar materials with perfect and/or imperfect contact conditions. To verify the formulation, several examples are provided here and the results from the numerical calculations are compared with the exact analytical solution. The problem chosen is steady-state heat flow in three zones with a temperature of three at one end and zero at the other end; adiabatic condition is applied to the other four surfaces. The 2-D cross-section of the configuration for this problem is shown in Figure 3. In all problems, the thermal conductivity of the first and the third zones are assumed to be equal. This problem was chosen because it was used in Reference 3; however, the exact solution provided there is incorrect. The correct solution for steady-state heat transfer in three zones with no resistance to the flow

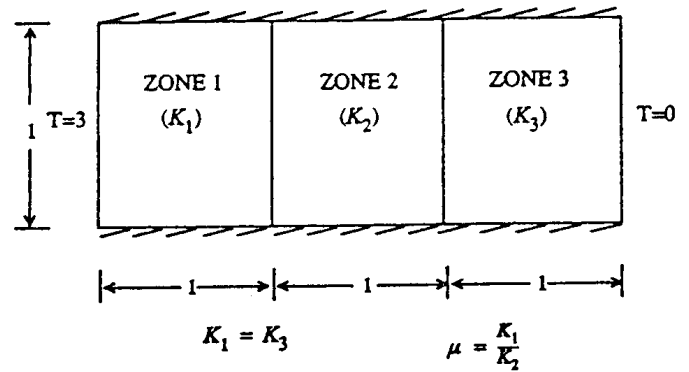


Figure 3. Configuration for steady-state heat transfer in three zones

of heat at the interfaces is [9]

$$T = \begin{cases} \frac{-3}{\mu+2}(x-\mu-2) & \text{for } 0 \leq x \leq 1 \\ \frac{-3}{\mu+2}(\mu x - 2\mu - 1) & \text{for } 1 \leq x \leq 2 \\ \frac{-3}{\mu+2}(x-3) & \text{for } 2 \leq x \leq 3 \end{cases}$$

where  $\mu = k_1/k_2$ . The exact solution to this problem can be generalized by including the resistance to the flow of heat at the interfaces between zones, i.e.,

$$T = \begin{cases} \frac{-3}{2+\mu+\alpha+\beta}(x-\mu-\alpha-\beta-2) & \text{for } 0 < x \leq 1 \\ \frac{-3}{2+\mu+\alpha+\beta}(\mu x - 2\mu - \beta - 1) & \text{for } 1 < x < 2 \\ \frac{-3}{2+\mu+\alpha+\beta}(x-3) & \text{for } 2 < x \leq 3 \end{cases}$$

where  $\mu = k_1/k_2$ ,  $\alpha = k_1/h_1$ ,  $\beta = k_1/h_2$ ,  $h_1$  is the conductance (inverse of the resistance) at the interface between the first and the second zones, and  $h_2$  is the conductance at the interface between the second and the third zones. As expected, the previous solution is recovered when there is no resistance at the interfaces (i.e., when  $\alpha = \beta = 0$ ).

A total of 256 "piecewise-constant" rectangular elements were used to discretize the exterior surface and

the two interfaces leading to a total of 288 DOFs for the case of resistance at the interface and 256 DOFs when interfaces are in perfect contact. The resistance at the interface between subdomains is defined to be proportional to the thickness of plate elements which are used to model the interface between subdomains (a zero plate thickness indicates perfect contact between subdomains). This resistance is computed by dividing the thickness by the thermal conductivity of the gases which fill the gap. Only the mid-plane of the gap between subdomains is modeled (recall that elements on the

interface have two faces). The connectivity tables and a simplified ray-tracing procedure are used to determine the orientation and the corresponding material on either side of the elements on this mid-plane.

In the first example,  $\mu = 10$  and the resistance at the interfaces between zones requires two DOFs at each node there, with  $\alpha = 4$  and  $\beta = 4$ . In the second example,  $\mu = 1$  (i.e., similar materials in all three zones), the resistance at the interfaces is maintained, with  $\alpha$  and  $\beta$  having the same values as in the first example. The results are shown in Figures 4 and 5, respectively. The

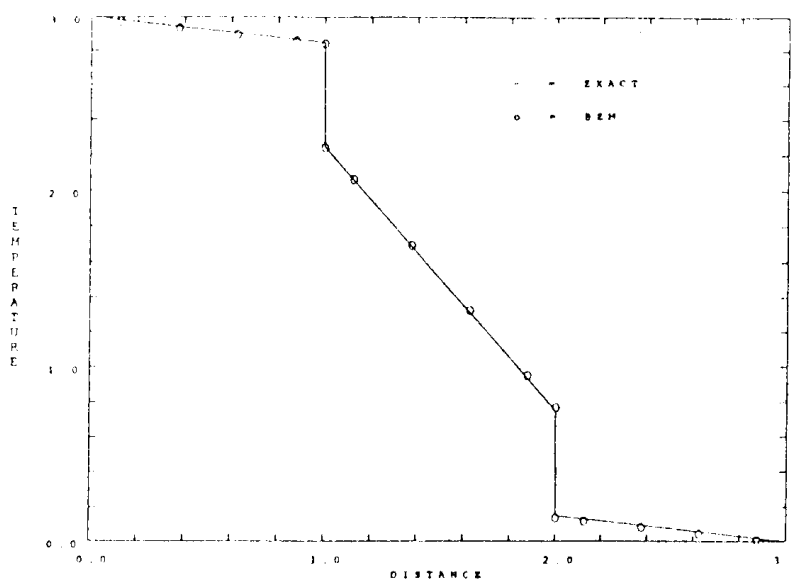


Figure 4. Temperature variation in three zones: Resistance at the interface between dissimilar materials ( $\mu = 10$ ,  $\alpha = 4$ , and  $\beta = 4$ )

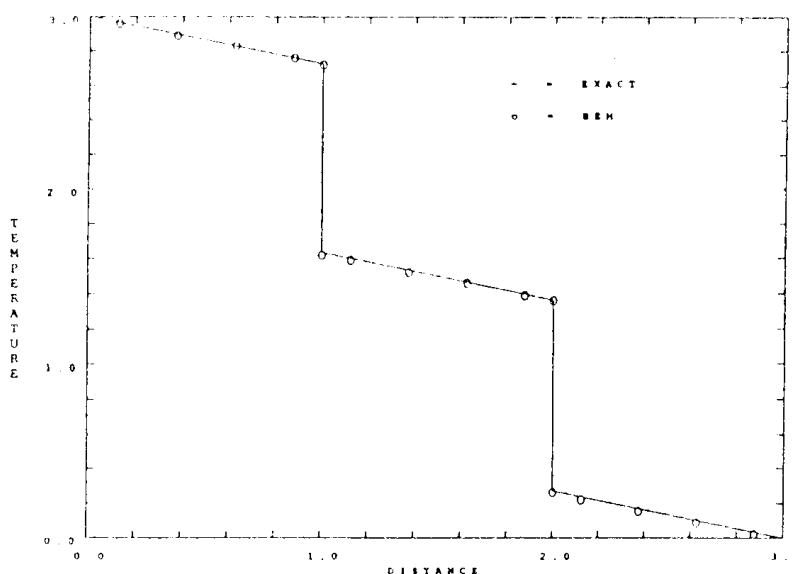
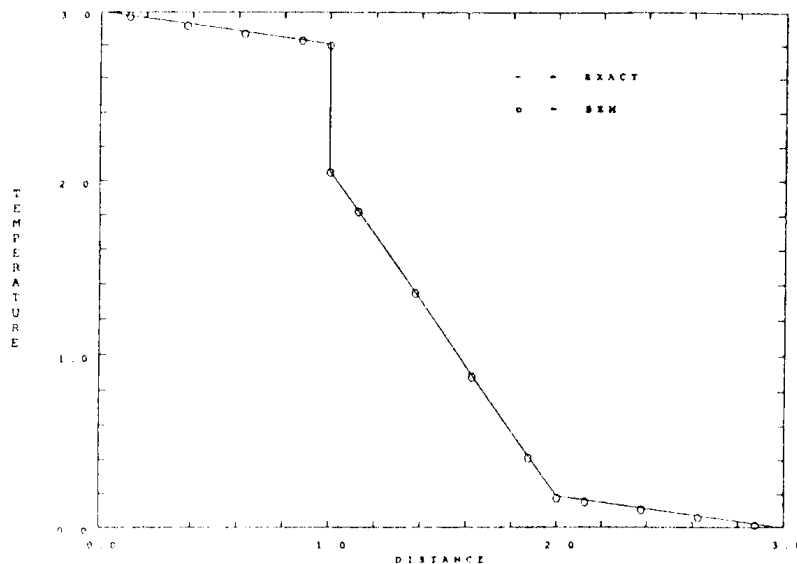


Figure 5. Temperature variation in three zones: Resistance at the interface between identical materials ( $\mu = 1$ ,  $\alpha = 4$ , and  $\beta = 4$ )



**Figure 6.** Temperature variation in three zones: Resistance at only one interface between dissimilar materials ( $\mu = 10$ ,  $\alpha = 4$ , and  $\beta = 0$ )

final example illustrates the mixture of gap and no-gap element formulations by allowing resistance at only one of the two interfaces. (Only one degree-of-freedom is required at each node on the perfect-contact interface.) The results are shown in Figure 6. It is observed that analytical and numerical results for all four problems are in excellent agreement even though a piecewise-constant approximation was used to generate the numerical results.

## CONCLUSIONS

The formulation presented here has combined the boundary formula, its gradient, and the exterior formula to solve steady-state heat transfer problems in piecewise homogeneous domains with general conditions at the interfaces between subdomains. The resulting integral equations lead to a sparse and well-conditioned matrix of coefficients with the minimum number of equations. A major advantage of this formulation over the existing methods is that any linear relationship for the conditions at the interface can be built into the integral equations at the outset, which allows generalizing the application of the Boundary Element Method for zoned problems. Another advantage is that the elements on the

interface between subdomains may be oriented in an arbitrary manner since the direction of the normal at any point on the interface is built into the integral equations. Also, no special numbering technique is required to obtain a banded system even though the matrix generated with the new algorithm is sparse. Finally, the modeling of the interfaces is simplified since only the midplane surface at an interface is discretized and the elements on this interface can have arbitrary orientation.

The formulation presented here has been validated as part of I-DEAS Mold Cooling, a commercial software program. (I-DEAS Mold Cooling is a trademark of Structural Dynamics Research Corporation.) Special formulations and procedures have enabled us to analyze efficiently and accurately the cooling cycle in injection molds made of several materials.

## REFERENCES

1. C. A. Brebbia, J. C. F. Telles and L. C. Wrobel, "Boundary Element Techniques, Theory and Application in Engineering", Berlin, Springer-Verlag, (1984).
2. J. D. Zheng, "Location of Free Surface for Zoned



- Problems-A New Economical Boundary Element Method", in *Boundary Elements, Proc. Fifth Int. Conf. on Boundary Elements*, C. Brebbia and Others, (Eds.), Hiroshima, Japan, (1983), pp. 85-94.
3. D. E. Medina, M. H. Lean and J. A. Liggett, "Boundary Elements in Zoned Media: Direct and Indirect Methods": *International Journal for Numerical Methods in Engineering*, Vol. 29, (1990), pp. 1772-1735.
  4. M. Rezayat, "A Novel Approach for Fast Decomposition of Boundary Element Matrices": in *Advances in Boundary Elements Methods in Japan and USA*, Computational Mechanics Publications, (1990).
  5. M. Rezayat and T. E. Burton, "A Boundary-Integral Formulation for Complex Three-Dimensional Geometries": *International Journal for Numerical Methods in Engineering*, Vol. 29, (1990), pp. 263-273.
  6. F. J. Rizzo, D. J. Shippy and M. Rezayat, "A Boundary Integral Equation Method for Radiation and Scattering of Elastic Waves in Three Dimensions": *International Journal for Numerical Methods in Engineering*, Vol. 21, (1985), pp. 115-129.
  7. A. J. Burton and G. F. Miller, "The Application of Integral Equation Methods to the Numerical Solution of Some Exterior Boundary-Value Problems": *Proceedings of the Royal Society of London A*, Vol. 323, (1971), pp. 201-210.
  8. C. Schwab and W. L. Wendland, "On Numerical Cubatures of Singular Integrals in Boundary Element Methods": *Math. Inst. A, Univ. Stuttgart*, (1991), Preprint 91-3.
  9. M. Rezayat, "Letter to the Editor on D. E. Medina et. al. Paper": *International Journal for Numerical Methods in Engineering*, (1991), To be published.