**Conference paper**
Dawson, M, Borman, DJ, Hammond, R, Lesnic, D and Rhodes, D *Predicting a Time Evolving Accumulating Crystalline Formation using a Meshless Boundary Tracking Approach.* In: Particle Systems Analysis PSA2011, 05 Oct 2011 - 07 Oct 2011 , Hilton Grosvenor Hotel, Edinburgh, UK.

# Predicting a Time Evolving Accumulating Crystalline Formation using a Meshless Boundary Tracking Approach

Michael Dawson[1], Duncan Borman[1], Robert Hammond[1], Daniel Lesnic[2] and Dominic Rhodes[3]

1. School of Process, Environmental and Materials Engineering, University of Leeds Leeds LS2 9JT, UK, pm09mcd@leeds.ac.uk
2. Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK. amt5ld@maths.leeds.ac.uk,
3. National Nuclear Laboratory, Central Laboratory, Sellafield, Seascale, Cumbria CA20 1PG, UK, dominic.rhodes@nnl.co.uk

## ABSTRACT

*The work presented attempts to construct a thermal imaging method with potential for numerically detecting the deposition of solidifying industrial process liquors evolving through time. In this simplified case it is assumed that the physical problem can be described by the two-dimensional time dependent heat equation. The problem is then posed mathematically, as an inverse geometric problem, which is solved numerically using the meshless Method of Fundamental Solutions (MFS). This allows the reconstruction of an internal boundary that describes the shape of the solidifying deposit as it develops through time. The main advantage of this method is that only non-invasive data is required, such as wall temperatures and heat fluxes. Numerical results presented correspond to a possible formation occurring due to an industrial pipe leakage.*

**Keywords**, Inverse Problem, Thermal Imaging, Method of Fundamental Solutions, Crystallisation

## 1. INTRODUCTION

The ability to non-invasively monitor and detect the development of solidifying process liquor is vital within many industrial applications. Undetected build up of such liquors, usually brought about by equipment malfunction or containment vessel failures, can potentially lead to hazardous conditions. With sufficient reliable monitoring procedures these situations can be minimised and detected quickly. This holds true for a variety of industries and in particular for the nuclear industry where knowledge of the size, shape and morphology of fissile material is critical, as undesirable conditions may potentially pose a large safety risk. The radioactive nature of these materials makes it challenging to use manual inspection as human exposure should be kept to a minimum or even non-existent when dealing with highly active liquors. Furthermore, most electronic inspection equipment cannot operate reliably within close proximity for extended periods of time.

The work presented within the paper attempts to address the problems outlined by constructing and evaluating non-invasive thermal imaging method. The fundamental principle behind the approach, is that a meshless numerical method is implemented, namely the Method of Fundamental Solutions (MFS), in order to solve the two-dimensional time dependent heat equation. Formulating this mathematically as an inverse geometric problem allows the reconstruction of an internal time dependent boundary which allows the non-invasive mapping of developing internal structures through time.

A range of experiments were conducted by the National Nuclear Laboratories (NNL), using a simulant solution of Sodium Nitrate in order to further understand dripping crystalline materials under a range of environmental conditions. An example of the type of formations that could form is shown in Figure 1. In order to test the numerical method, attempts are made to use the approach to locate standardised geometric inclusions based on simplified morphologies from external boundary information (temperatures and heat flux).

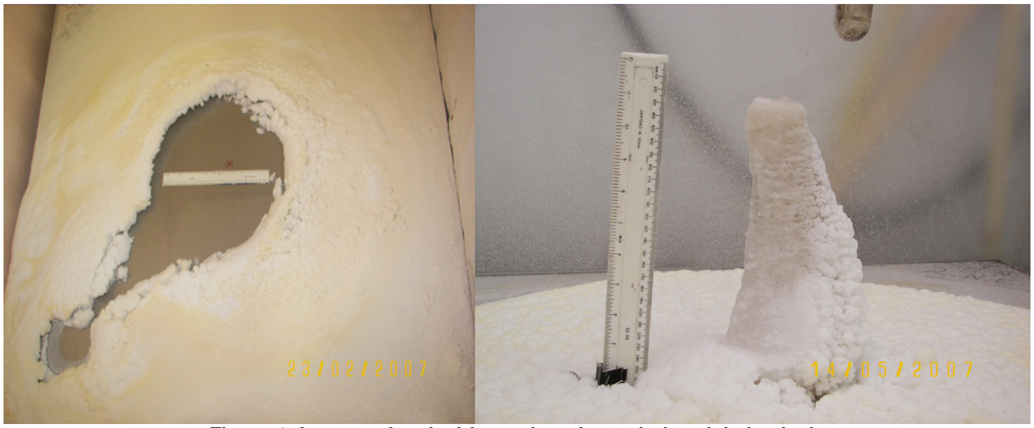


**Figure 1: Images of typical formations for an industrial pipe leak.**

## 2. MATHEMATICAL MODEL AND NUMERICAL SOLUTION

The mathematical formulation of the inverse geometric problem under investigation requires finding the temperature $u$ and the moving internal defect $D(t)$ compactly contained in a spatial planar bounded domain $\Omega$ such that $\Omega \setminus D(t)$ is connected satisfying the two-dimensional time-dependent heat equation

$$\frac{\partial u}{\partial t}(x,t) - \Delta u(x,t) = 0, \quad (x,t) \in (\Omega \setminus \overline{D(t)}) \times (0,T], \quad (1)$$

subject to the outer wall temperature (2), the inner inclusion boundary temperature (3), the initial (4) conditions

$$u(x,t) = f(x,t), \quad (x,t) \in \partial\Omega \times [0,T], \quad (2)$$

$$u(x,t) = h(x,t), \quad (x,t) \in \partial D(t) \times [0,T], \quad (3)$$

$$u(x,0) = u_0(x), \quad x \in \overline{\Omega} \setminus D(0), \quad (4)$$

and the additional heat flux measurement

$$\frac{\partial u}{\partial n}(x,t) = g(x,t), \quad (x,t) \in \partial\Omega \times [0,T], \quad (5)$$

where $\underline{n}$ is the outward normal to the boundary. For a unique solution we assume that the initial domain *D(0)* is known.

By using the Method of Fundamental Solutions (MFS) we seek an approximate solution as a linear combination of non-singular fundamental solutions, see Johansson *et al.* (2011),

$$U_{M,N}(x,t) = \sum_{m=1}^{2M} \sum_{j=1}^{2N} c_j^m F(x,t; y_j^m, \tau_m), \quad (x,t) \in (\overline{\Omega} \setminus D(t)) \times [0,T], \quad (6)$$

where $(y_j^m)_{j=\overline{1,2N}}^{m=\overline{1,2M}}$ are space 'singularities' (sources) located outside the space domain $\overline{\Omega} \setminus D(t)$, $\tau_m$ are times located in the interval $(-T,T)$, and $F$ is the fundamental solution for the two-dimensional heat equation given by

$$F(x,t;y,\tau) = \frac{H(t-\tau)}{4\pi(t-\tau)} \exp\left(-\frac{|x-y|^2}{4(t-\tau)}\right). \quad (7)$$

As the boundary and initial conditions (2)-(5) are known we can fit the approximated data of the MFS to these values using a nonlinear least-squares formulation to find the unknown values the unknown vector of coefficients $\underline{c}$ and the star-shaped defect $D(t)$ which is assumed to be parameterised by an unknown vector of radii $\underline{r}$. This recasts into the minimization of the following least-squares functional:

$$S(\underline{c},\underline{r}) = \| U_{M,N} - f \|^2 + \| U_{M,N} - h \|^2 + \| \frac{\partial U_{M,N}}{\partial n} - g \|^2 + \| U_{M,N} - u_0 \|^2 . \quad (8)$$

A minimisation process is then performed on the objective function (8) using the MATLAB routine 'FMINCON' in order to fit the MFS approximation to known data.

The physical set up of the above method is shown in Figure 2. Here we take a circular domain $\Omega$ for simplicity. In the MFS, *N* sensors (collocation points) are placed uniformly across the outer wall and readings are taken for *M* intervals in time. More details of the MFS implementation can be found in Dawson *et al.* (2011).

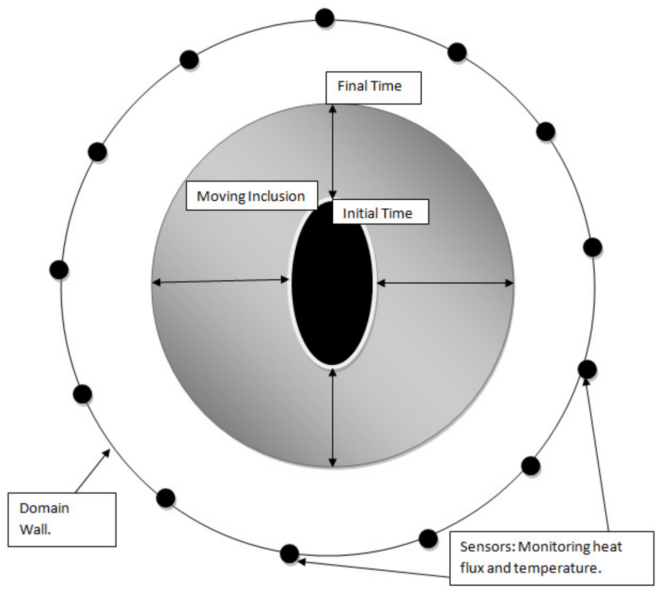


**Figure 2. Physical set-up for the method described in section 2.**

## 3. NUMERICAL RESULTS

Initially, the method has been tested by the authors for identifying simple geometries successfully (e.g. circular inclusions). Here we attempt to locate a peanut star-shaped boundary $D(t)$, parameterised by,

$$r(\theta) = \frac{2}{3}\sqrt{\cos^2\theta + 0.26(\sin\theta + 0.25)^2}. \quad (9)$$

We take *T*=1 and the boundary and initial conditions (2)-(4) given by

$$u(x,t) = f(x,t) = t, \quad (x,t) \in \partial\Omega \times [0,T],$$
$$u(x,t) = h(x,t) = 0, \quad (x,t) \in \partial D(t) \times [0,T],$$
$$u(x,0) = u_0(x) = 0, \quad x \in \overline{\Omega} \setminus D(0),$$

and we generate the heat flux data (5) numerically by solving first, using the MFS, the direct problem given by equations (1)-(4) when the inclusion *D(t)* is known and given by equation (9). The temperature and heat flux values are not based on experimental values in this example, since it is the purpose of this paper to evaluate the proposed method, therefore taking cases with known solutions allows a direct comparison to be made with the calculated results. The geometry of the external domain is based around a circle of radius one metre and the time period taken arbitrarily as one hour.

Here the temperature and heat flux values are taken across $N$=18 uniform points on the domain boundary (wall) at $M$=18 equally spaced points in time, these have found to provide an adequate balance between computational time, accuracy and stability. The initial guess for the rigid inclusion is taken as a circle of radius 0.7. We also take $\underline{c}=\underline{0}$ as the initial guess for the vector of MFS coefficients.

Figures 3 displays the RMS and the objective function (8), where the RMS takes the form,

$$RMS=\sqrt{\frac{\sum_{j=1}^{N}\sum_{m=0}^{M}(r_j^m-r_j^*)^2}{N(M+1)}},\quad (10)$$

where $r_j^m$ are the discrete radial values for the radius $r(\theta,t)$, which parameterises the unknown inclusion $D(t)$ and $r_j^*$ are the discrete values of the exact inclusion (9).

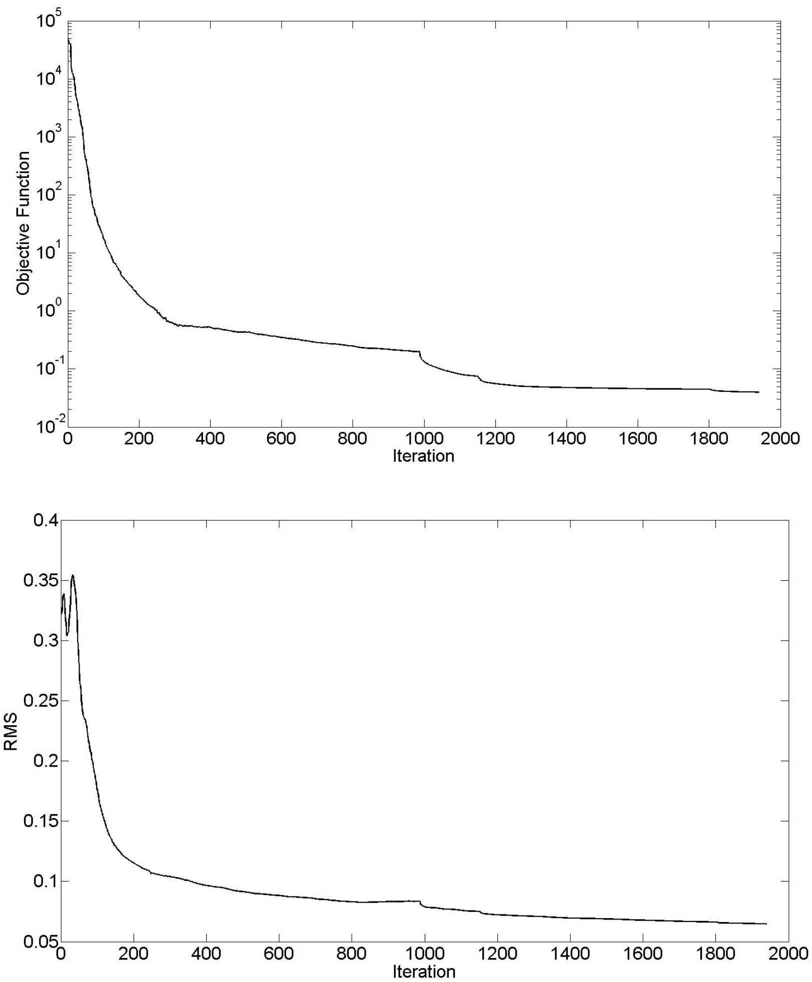


**Figure 3. Objective Function (8) and RMS (10) for various iterations.**

The numerical solution at the final time, $t=T=1$, and the full space-time plot are shown in Figure 4. From this figure it can be seen that in the case of this relatively complex geometry the MFS provides a good approximation of the unknown inclusion, *D(t)*. In this example the unknown shape does not move in time, however this is not know *a priori* so it provides a suitably robust case in order to test the method. More work has been conducted to investigate the retrieval of inclusions where geometries change over time. These have also been successfully located using the proposed approach.

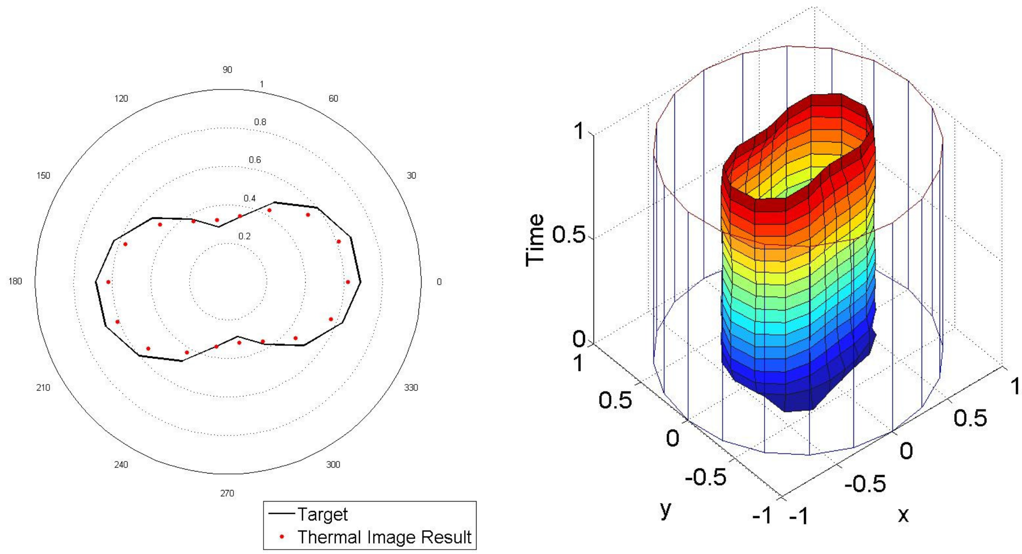


**Figure 4. Plot of the final solution at $t=T=1$ and space-time plot of the inclusion located using the approach.**

## 4. CONCLUSIONS

This paper has demonstrated the use of the proposed method for one example. The method was shown to be reasonably accurate for a fairly complex stationary shape. Results will be shown at the conference for reconstructing time-dependent shapes with noisy data.

## ACKNOWLEDGEMENTS

The authors would like to thank both the ESPRC and National Nuclear Laboratory for continual funding and support.

## REFERENCES

**1.** M. Dawson, D. Borman, R. Hammond, D. Lesnic and D. Rhodes (2011) Meshless detection of an internal moving boundary, *Proc. 8th UK Conf. Boundary Integral Methods*, (ed. D. Lesnic), Leeds University Press, pp.17-24.

**2.** B.T. Johansson, D. Lesnic and T. Reeve (2011) A method of fundamental solutions for two-dimensional heat conduction, *International Journal of Computer Mathematics*, **88**, 1697-1713.