JOURNAL OF APPLIED
COMPUTER SCIENCE
Vol. 19 No. 2 (2011), pp. 111-123

Possibility to Use the Diffusion Equation to Heat Flow Modeling in a Composting Process

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Abstract. *The paper proposes a new concept to use the diffusion equation for heat flow estimation in a composting process. Only general ideas are described, without the full mathematical model and without experiments. The lack of the detailed description stems from the fact that such an approach was not (as it seems) used earlier, and the details are to be developed. The article describes the preparatory work in this field. In the first part of the article, derivation of the diffusion equation is presented together with using an approach consistent with modern Computational Fluid Dynamics, in which all fluid phenomena in a Control Volume are considered. In the second part of this article, the basic information about implementation and needed programming techniques are described. It is emphasized that the diffusion equation is adequate not only for the temperature flows, but for other phenomena as well. The main purpose of this study is to create a general template for 3D modeling of phenomena which are diffusive in nature.*
Keywords: *compost, low-temperature heat source, heat flow, diffusion equation, CFD.*

1. Introduction

Composting is a semi-natural degradation process for matter of plant origin. During this process heat is generated, which can then be drained off and used.

Numerous studies indicate that after a dozen or tens of hours after the beginning of composting there followed a significant rise in temperature in the compost volume. This is due to the growing population of bacteria. It is important that the bacteria do not grow uniformly throughout the volume but occur locally at various points. Then the multiplication and spread of bacteria is in progress. After the extreme, the temperature drops slowly to the temperature of the surroundings within a few weeks. This process is known and described in many works, such as e.g. [1], [2], [3], [4]. Of course, the specific values of temperature and time of heat generation depend on the particular case and may change significantly. However, for some time the temperature is high enough to serve as a low-temperature heat source [5], [6], [7].

In the literature we can find studies related to modeling of compost behavior. The mathematical model depends on the individual objectives of the authors, but usually the distribution of temperature in time, and less, in space, plays in it the key role. Chad et al [8] in their work develop a mathematical model based on balances of moisture, oxygen mass fraction and temperature. Kaiser [9] shows a model in which the equilibrium of carbon dioxide, water and temperature is considered. In Weppen work [4] the heat fluxes, flowing from the vessel to the surroundings, are the basis of the mathematical model. Heat balance was discused in papers [1], [10] and other. After this review we can assume that in the composting process without aeration the temperature distribution depends primarily only on a few scalar variables. It is important that those variables should be functions of time and location in space. It is best to define these variables as scalar fields.

Treating the compost as a low-temperature heat source, the time and spatial temperature distribution are the key issue. The main idea presented in this article is to use the so-called diffusion equation to the calculation of the temperature distribution in time and space, simultaneously. It seems that in the literature this approach to the modeling of the composting process is not used. It should be emphasized that in this article we do not present a mathematical model of compost behavior - it is only a "template", which can serve to develop a new computational 3D model. We focus on the general features of the diffusion equation, numerical, programming and visualization issues. The final refinement of the simulation model will be possible after obtaining reliable experimental data, which is planned for the future. The motivation to begin studies in this field was a discussion conducted on a conference during which there appeared the idea of the application of diffusion equation in the field of research on the use of heat formed in the composting process. The article describes the preparatory work in this field.

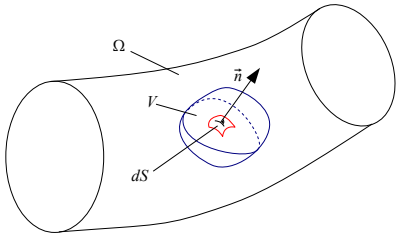

Figure 1. A Control Volume

In the first part of the article derivation of the diffusion equation is presented. This derivation differs from the classical way but the used approach is consistent with modern Computational Fluid Dynamics, in which all fluid phenomena in a Control Volume are considered. In the second part of this article the basic information about implementation and needed programming techniques are described. All the time it is emphasized that the diffusion equation is adequate not only for the temperature flows, but for other phenomena as well. For this reason all equations are based on the general variable Φ, which can be interpreted in several ways. We want to emphasize the universality of the developed computational mechanism and hope that the reader finds his own applications.

2. General form of the diffusion equation

Consider a Control Volume $V \in \Omega$ closed by a surface S (Fig. 1). Let ϕ denote density of a physical quantity Φ flowing througth the space Ω. The change rate of quantity inside the volume V in the time interval dt is equal to the sum of fluxes $\vec{\phi}$ of this quantity, flowing through the surface S in perpendicular direction:

$$\frac{d}{dt}\int_V \Phi dV = -\int_S (\vec{\phi}\cdot\vec{n})dS, \tag{1}$$

where $\vec{n}$ is the versor of the surface S. The positive sign applies to the effluent flux from the volume, hence the negative sign in the formula.

The formula (1) can be written in other form by using the Green-Gauss-Ostrogradzki Theorem [11], [12], [13]. Now the surface integral will be changed into the volume integral as follows

$$\frac{d}{dt}\int_V \Phi dV = -\int_V div(\vec{\phi})dV. \tag{2}$$

The left-hand side of equation (2) may be transformed using the Reynolds Transport Theorem [13] and next the Green-Gauss-Ostrogradzki Theorem to the form

$$\frac{d}{dt}\int_V \Phi dV = \int_V \frac{\partial \Phi}{\partial t}dV + \int_S (\Phi\vec{v}\cdot\vec{n})dS = \int_V \frac{\partial \Phi}{\partial t}dV + \int_V div(\Phi\vec{v})dV. \tag{3}$$

The above formula has a very general form, including cases in which the material - which is a carrier of the physical quantity Φ - is moved (it is also a fluid). If the lifting speed $\vec{v}$ is equal to zero, it may be written

$$\frac{d}{dt}\int_V \Phi dV = \int_V \frac{\partial \Phi}{\partial t}dV. \tag{4}$$

After substituting (4) to (2) we obtain

$$\int_V \frac{\partial \Phi}{\partial t}dV = -\int_V div(\vec{\phi})dV \tag{5}$$

or

$$\int_V \Big[\frac{\partial \Phi}{\partial t} + div(\vec{\phi})\Big]dV = 0. \tag{6}$$

Integral will be zero, only if the integrand expression zeroed

$$\frac{\partial \Phi}{\partial t} + div(\vec{\phi}) = 0. \tag{7}$$

It is worth noting that the equation (7) has its very good counterpart in the fluid mechanics. If the quantity Φ represents the density ρ of a fluid, we obtain the classical equation of mass balance [14]

$$\frac{\partial \rho}{\partial t} + div(\rho\vec{v}) = 0. \tag{8}$$

where $\rho\vec{v}$ is the mass flux of the fluid. If the flux $\vec{\phi}$ is proportional to the gradient of Φ, the expression (7) obtains its form

$$\frac{\partial \Phi}{\partial t} + div(-\alpha \cdot \nabla \Phi) = 0. \tag{9}$$

or

$$\frac{\partial \Phi}{\partial t} - \alpha \cdot \nabla^2 \Phi = 0, \tag{10}$$

where α is a proportionality factor.

Depending on the interpretation of individual variables, equation (10) can describe several issues in physic, for example the problem of equalizing the temperature based on the Fourier law [15], [16], [17], [18], [19]:

$$\vec{q}_T = -\lambda \cdot \nabla T, \tag{11}$$

where T is the temperature $[K]$, $\vec{q}_T$ is the heat flux $[W/m^2]$, and λ is the heat conductivity $[W/(m \cdot K)]$. According to the Fourier Law, the equation (10) obtains now the so-called heat equation form

$$\frac{\partial T}{\partial t} - \lambda \cdot \nabla^2 T = 0. \tag{12}$$

Other example of the application the formula (10) can be the problem of equalizing the concentration of a component based on the first Fick Law [20], [21], [19]:

$$\vec{j}_C = -\rho \cdot D \cdot \nabla C, \tag{13}$$

where $\vec{j}_C$ is the molar diffusion flux $[mol/(m^2 \cdot s)]$, ρ is the density $[kg/m^3]$, D is the diffusion coefficient $[m^2/s]$ and C is a concentration of the component. In this case, the formula (10) can be written as follows:

$$\frac{\partial C}{\partial t} - \rho \cdot D \cdot \nabla^2 C = 0. \tag{14}$$

The diffusion equation can also be used for modeling the concentration of carriers in semiconductors, Markov processes and other phenomena.

3. Implementation of the diffusion equation

The calculation space Ω was adopted as a cube with length L_x, L_y and L_z. For this shape the Cartesian coordinates and structured grid are convenient. The spatial grid steps can be calculated from the formulas

$$dx = \frac{L_x}{n_x}; dy = \frac{L_y}{n_y}; dz = \frac{L_z}{n_z} \tag{15}$$

where: n_x, n_y and n_z denote number of cells in directions x, y and z, respectively.

In 3D Cartesian space, the equation (10) obtains the form [15], [22], [23], [24]

$$\frac{\partial \Phi}{\partial t} = \alpha \cdot \left(\frac{\partial \Phi}{\partial x} + \frac{\partial \Phi}{\partial y} + \frac{\partial \Phi}{\partial z} \right). \tag{16}$$

With using the Euler scheme for time discretisation [25], [26], [27] we obtain:

$$\frac{\Phi^{n+1} - \Phi^n}{\Delta t} = \alpha \cdot \left(\frac{\partial \Phi}{\partial x} + \frac{\partial \Phi}{\partial y} + \frac{\partial \Phi}{\partial z} \right). \tag{17}$$

where the subscript n denotes current time level. New value of quantity Φ in time level $n + 1$ can be also calculated for formula (17)

$$\Phi^{n+1} = \Phi^n + \alpha \cdot \left(\frac{\partial \Phi}{\partial x} + \frac{\partial \Phi}{\partial y} + \frac{\partial \Phi}{\partial z} \right) \cdot \Delta t. \tag{18}$$

In case of three dimensional structured grids (Fig. 2) and an explicit forward in time, central in space method [22], [24] we obtain

$$\begin{cases} \Phi^{n+1}_{i,j,k} = \Phi^n_{i,j,k} + \alpha \cdot \left(\frac{\Phi^n_{i+1,j,k} - 2\Phi^n_{i,j,k} + \Phi^n_{i-j,j,k}}{dx^2} + \right. \\ \left. + \frac{\Phi^n_{i,j+1,k} - 2\Phi^n_{i,j,k} + \Phi^n_{i,j-1,k}}{dy^2} + \frac{\Phi^n_{i,j,k+1} - 2\Phi^n_{i,j,k} + \Phi^n_{i,j,k-1}}{dz^2} \right) \cdot \Delta t. \end{cases} \tag{19}$$

where $\Phi^n_{i,j,k}$ is the local in space and time value of balanced quantity Φ. The subscript contains information about the location of cells in the grid. The solution for this scheme is conditionally stable, based on the CFL number.

In the general case, the proportionality factor can be a function (scalar field) depending on the balanced quantity Φ, calculation time t and other parameters

$$\alpha_{i,j,k} = f(\Phi, t, ...) \tag{20}$$

To the calculation of changes of the value Φ, spatial difference of this quantity is needed. It can be achieved by adding the scalar field of heat source S to the model. In the case of composting, these sources represent places in space from

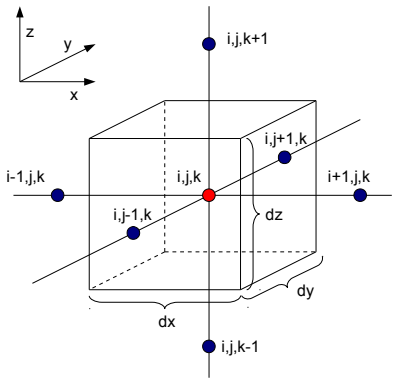

Figure 2. A numerical grid cell

which begins the process of multiplication of bacteria. An adequate theory must be here developed, but in the general case these sources may depend on the position in space, time and other parameters

$$S_{i,j,k} = f(\Phi, t, ...). \tag{21}$$

Other parameters in equations (20) and (21) can be any variables that may affect phenomena in composting process. These could be scalar fields of porosity, moisture or water content, oxygen content, carbon dioxide content or other factors. The number of those scalar fields is unlimited.

To the resolving the diffusion equation in 3D space we used Fortran 90/95 programming language (GNU gfortran compiler and own programming environment [28]), specifically designed for mathematical computation. In the developed software, the formula (19) was used. On the boundary of the calculation space Ω, the Dirichlet boundary condition was defined. The results of calculation were saved in VTK file format [29] and next imported in ParaView software [30].

An example of result calculation in which the quantity Φ is interpreted as the temperature is shown in Fig. 3. In this case tens of heat sources were manually defined. These sources operate at different times and varied in intensity. Therefore, the temperature was changing throughout the volume of the compost: first increased (hotter areas grow by the action of sources) and later decreased (the number of sources decreases and they have lower values). Additionally, it was assumed

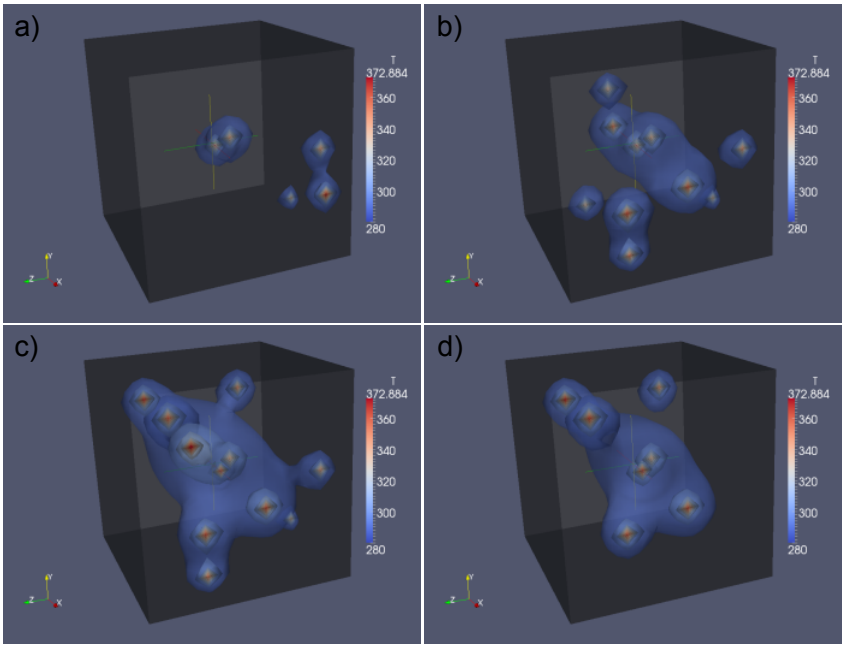

Figure 3. Space distribution of the quantity Φ on four different time levels: a) 50 h, b) 100 h, c) 200 h, d) 250 h

that the value of the proportionality factor α is a sum of the main value, described by a function, and disruptions. Those disruptions were modeled by using a random function: the initial scalar field of the proportionality factor is presented in Fig. 4. In this way, the properties of the balanced quantity carrier are not uniform, just as in real compost. In the presented case, the initial value of temperature field was constant and equal to 280$[K]$, the main value of the proportionality factor α was 5.0, and the total calculation time was 400 hours.

In the course of the calculations we also tracked the average value of all defined scalar fields. In this way the results of calculations can be compared with the literature. The average temperature for all volume of compost is shown in Fig. 5. The total temperature increment is here relatively small due to a small number of sources. In the real systems this increment must be much larger because almost in the whole volume of the compost the heat is generated. The other difference is that the value of sources in real systems is lower than in this test case. The exact

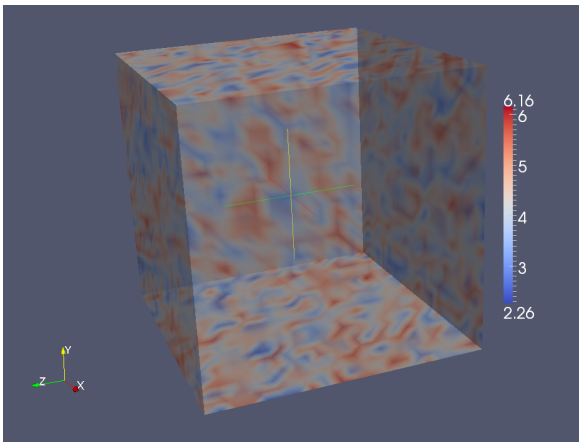

Figure 4. Initial space distribution of the proportionality factor α

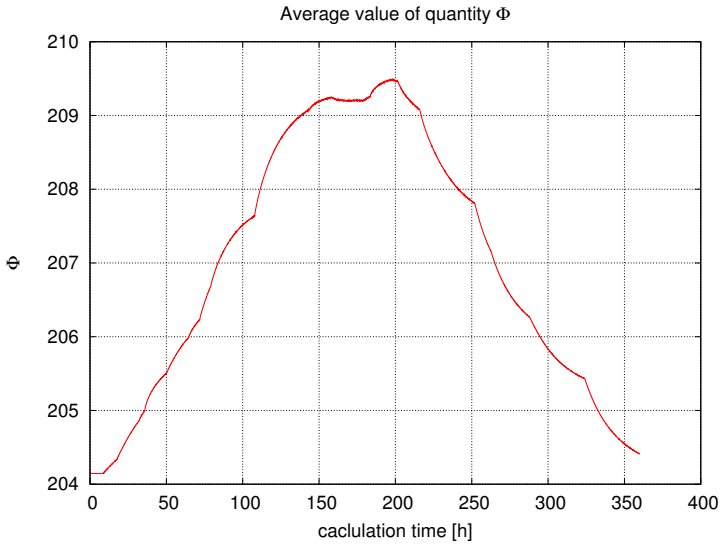

Figure 5. Average value of the quantity Φ in time function

description of these values sets the direction for further investigations. However, the overall trend of temperature changes is in line with expectations.

4. Summary

In the article a general numerical model for diffusion phenomena was described. The author hopes that after further investigations it can be used for calculation of heat distribution in a composting process. This will be possible when the experimental data will be available. The main goal for the future is to replace the manual definition of sources by a mathematical model, according to the formula (21). The properties of the heat carrier must be described as well by appropriate "closures".

It was mentioned at the beginning that the ultimate goal of investigations is to devise a method of receiving the heat which is generated during the composting process. The numerical mechanism described in the article allows doing it. The heat receiver (e.g. in the form of pipes) can be modeled here as a "negative heat source". This source must be local in nature and correspond to the location of such pipes of heat exchanger. This phase is planned later, after developing the details of the basic mathematical model.

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