



Co-published by  
**Institute of Fluid-Flow Machinery**  
Polish Academy of Sciences  
**Committee on Thermodynamics and Combustion**  
Polish Academy of Sciences

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## Issues on numerical modelling of transport processes in granular reactive media – an approach with thermal relaxation

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Received: 14.02.2024; revised: 24.06.2024; accepted: 25.06.2024

### Abstract

The steadily growing interest in applying granular media in various novel and advanced technologies, particularly in the energy sector, entails the need to gain in-depth knowledge of their thermal and flow behaviour and develop simulation predictive tools for systems' design and optimisation. The focus of the present study is on the numerical modelling of the thermal decomposition of solid fuel grains in a packed bed while considering a non-classical description of heat transfer in such a medium. The work aims to assess the influence of the relaxation time and thermo-physical properties of the medium on the nature of the solution and highlight the factors that are the source of local non-equilibrium affecting thermal wave speed propagation. The analysis of the predicted temperature distribution was carried out based on the developed transient one-dimensional thermal and flow model, taking into account the moisture evaporation and the devolatilization of fuel particles. Obtained simulation results showed a significant increase in the temperature gradients with increased relaxation times for the case of wet granular bed. They also demonstrated the variable dynamics of thermal wave propagation due to the change in the packed bed structure with the process progress. For a relaxation time of 100 s, a several-fold increase in the temperature signal propagation speed during the fuel bed thermal decomposition was predicted.

**Keywords:** Reactive media; Granular material; Non-Fourier model; Relaxation time; Hyperbolic equations

Vol. 45(2024), No. 3, 5–12; doi: 10.24425/ather.2024.150450

Cite this manuscript as: Polesek-Karczewska, S., & Kardaś, D. Issues on numerical modelling of transport processes in granular reactive media – an approach with thermal relaxation. *Archives of Thermodynamics*, 45(3), 5–12.

### 1. Introduction

Granular materials have wide and growing applications in modern technologies, especially in the field of energy systems and devices. As filling porous materials, owing to their structure, they could offer far higher Nusselt numbers, and thereby increased heat transfer rates in the case of laminar flow, compared to non-filled flow spaces [1,2].

Recent advances involve the use of porous materials to enhance heat transfer in energy storage systems, such as shell-and-tube thermal energy storage (TES) units with composites in the form of multiple PCMs with alumina nanoparticles, or cascaded aluminium foam [3], or porous SiC/paraffin composite PCMs [4]. In thermochemical energy storage systems, porous materials are the constituents of composite thermochemical materials [5]. Fluid-saturated porous cavities are also the subject of extensive studies in terms of convection heat transfer in various cooling

## Nomenclature

$a$	– thermal diffusivity, $\text{m}^2/\text{s}$
$A, B$	– matrices of coefficients
$c$	– specific heat, $\text{J}/(\text{kg K})$
$\mathbf{c}$	– vector of source terms
$h$	– enthalpy, $\text{J}/\text{kg}$
$p$	– pressure, $\text{Pa}$
$\mathbf{q}$	– heat flux, $\text{W}/\text{m}^2$
$R$	– particle diameter, $\text{m}$
$t$	– time, $\text{s}$
$T$	– temperature, $\text{K}$
$V$	– velocity, $\text{m}/\text{s}$
$w^{(1)}, w^{(2)}$	– variables
$x$	– space coordinate, $\text{m}$
$\mathbf{y}$	– vector of unknowns

## Greek symbols

$\rho$	– density, $\text{kg}/\text{m}^3$
$\lambda$	– thermal conductivity, $\text{W}/(\text{m K})$

$\sigma$	– Stefan-Boltzmann constant, $5.67 \times 10^{-8} \text{ W}/(\text{m}^2 \text{ K}^4)$
$\xi$	– wave propagation speed, $\text{s}$
$\theta$	– relaxation time, $\text{s}$

## Subscripts and Superscripts

$c$	– conduction
$g$	– gas
$r$	– radiation
$s$	– solid
$sg$	– solid to gas
$w$	– water
$wg$	– water to gas
0	– initial

## Abbreviations and Acronyms

PCM	– phase change materials
TES	– thermal energy storage

applications in the area of electronics, solar and nuclear energy systems, or heat exchangers [6]. In addition, granular packed beds serve as the adsorption media in refrigeration devices [7]. Furthermore, axially graded porous materials have gained an interest in the context of cooling systems, where not only the required temperature but also its uniformity in the medium is of concern [8]. Following the efforts towards sustainable development through energy saving, pollution reduction, and the use of available alternative biogenic fuels, the common have become porous burners [9], which due to enhanced heat transfer ensures more efficient and stable combustion, and thus enables the combustion of low-grade fuels with low pollutant emission levels. Along with this, porous materials have also been considered in the context of direct-contact heat exchangers for flue gas heat recovery [10]. Therefore, modelling heat transfer in such media becomes one of the key aspects in predicting the performance of energy-efficient systems. This also refers to various technologies of thermal conversion of solid fuels. The description of transient heat transport in granular media such as reactive packed beds is a difficult issue due to all heat transport mechanisms being involved and the variability of the particle structure during the material physicochemical transformations that accompany its thermal conversion. During the process, the particles change shape, can swell, shrink, and fragment, but above all their porosity changes. These changes in structure significantly affect the dynamics of gas flow through the bed and its diffusion in the particles themselves, and thus the efficiency of phase transitions and chemical reactions. This may cause large local temperature differences between the solid and gas phases, reaching in the case of high-temperature processes even several hundred degrees [11]. Numerical analyses indicate that even for particles of relatively small size, with a diameter of a few millimetres, the predicted heating times of the particles when taking into account the intra-particle convection of water vapour and released pyrolysis gases are longer compared to the case with no convection

accounted for [12]. Due to non-uniform porosity distribution in packed beds of fuel particles, this effect can lead to local thermodynamic non-equilibrium.

The classical equilibrium description of transport phenomena in thermal-flow devices, based on Fick's, Newton's and Fourier's laws of gradient type, brings the issues to parabolic equations [13,14]. Their solutions demonstrate an instantaneous change in parameters at any point in the medium (e.g. temperature, pressure) in response to a change in parameters at another point in the medium. This nature of change is due to the assumed infinite speed of signal propagation, which is a non-physical effect. Closer to reality is the non-equilibrium approach, which introduces the hyperbolic-type equations for mass, momentum and heat fluxes. These take into account the relaxation times of the fluxes and thus satisfy the assumption of a non-zero propagation speed of disturbances [15].

Among the works regarding the non-classical, i.e. non-Fourier, description of heat transfer, theoretical analyses dominate. Following the need to account for the complex geometry, different boundary conditions and the variability of thermo-physical parameters, research has largely focused on numerical studies with the use of different solution methods [16]. It shall be noted that the limited number of experimental data in this area [17] significantly hinders the verification of the non-Fourier model predictions, leaving the question of the validity of its applicability to inhomogeneous materials still unresolved.

The literature review indicates that few works are dedicated to the analysis of the application of a non Fourier-type heat conduction model in the mathematical description of thermochemical processes. These include the works on combustion, both experimental [18] and theoretical [19], which point to the non-Fourier model as a more adequate description of heat transfer. This paper thus focuses on the numerical modelling of transport phenomena in a thermally processed reactive granular packed bed. The objective is to demonstrate the effect of variable structure-

related medium properties on the speed of a heat propagation wave. Based on the variant simulation results of a packed bed of solid particles undergoing thermal decomposition, the meaning of a relaxation time in the approach considered is discussed.

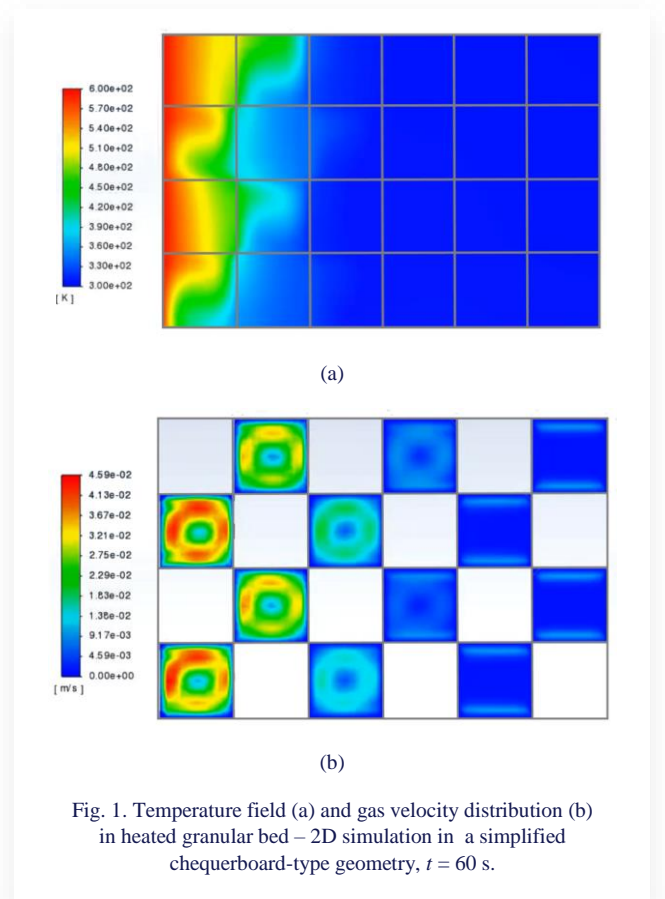
## 2. Modelling heat transfer in granular media

The classical heat conduction model, based on Fourier's law, is considered to sufficiently reproduce the characteristics of the heat transfer process in most engineering issues, also involving granular media when processes are slowly varying and heat pulses are small. However, due to the wave-like nature of the heat transfer [20], also in homogeneous materials, in processes of high dynamics and large thermal pulses, the predictions of the classical heat conduction model deviate significantly from the experimental data. Then, the problem description requires the use of an alternative model, proposed by Cattaneo and Vernotte, defining the heat flux as follows:

$$\mathbf{q} + \theta \frac{\partial \mathbf{q}}{\partial t} = -\lambda \nabla T, \quad (1)$$

where  $\lambda$  represents the thermal conductivity of a material,  $t$  is the time. Parameter  $\theta$  is the relaxation time, which is a key factor in the description that determines the delay of heat flux with respect to the temperature gradient. It is a function of the thermodynamic parameters of the medium and, thereby, is a variable quantity. The higher the temperature, the shorter the relaxation time. It is therefore recognised that a non-classical approach to heat transfer (Eq. (1)) should be used when the relaxation time is of an order of characteristic process time. proposed procedure is correct for the class of problems).

Experimental studies regarding granular media indicate much longer relaxation times compared to those reported for gases and solids and are of the order of a few to several seconds [19,21]. The reason behind this is a significant difference in heat transfer patterns through gas and solid phases. In engineering practice (e.g. pyrolysis reactors, gasifiers) the packed bed structure is complex, wherein the fuel particles are of irregular shape sizes with dimensions ranging from millimetres and centimetres. Nevertheless, just to highlight and visualize the possible occurrence of significant local temperature gradients in a two-component (solid/gas) reactive system, an example of non-homogeneous medium of a simplified geometry, heated on one side, may be considered, as illustrated in Fig. 1. The figure shows the temperature (Fig. 1a) and gas (air) flow velocity fields (Fig. 1b) in a chequerboard-type geometry (sized 6 cm × 4 cm) that represent a small section of the granular bed. It is composed of square solid elements (grey fields in Fig. 1b) and voids (closed cavities), each sized 1 cm × 1 cm. Though very simplified, such a case may mimic the densely packed granular (solid/air) bed of fuel particles with high flow resistance, to show the general thermal and flow patterns in such a system. The discussed computational case is two-dimensional and transient. Each element of the domain consisted of 100 cells (10×10). The thermo-physical properties of coal and air were adopted for the solid and voids, respectively. The initial temperature of the domain was set to



300 K and the stepwise increase of temperature to 600 K at the left boundary of the domain was assumed.

The simulation results displayed in Fig. 1a, showing the parameters' distribution after the 60 seconds of bed heating, clearly indicate the uneven temperature distribution in the packed bed cross-section transverse to the thermal wave propagation, which is due to the difference in thermal behaviour between the phases. As can be observed from the figure, the temperature differences in the granular bed cross-section may exceed 100 K. For the case considered, when comparing temperatures of the upper and bottom sub-layers, these differences may be estimated at ~150 K, 120 K and 70 K, at the cross-lines representing  $x = 0.5$  cm,  $x = 1$  cm, and  $x = 1.5$  cm, respectively. Obviously, the thermal front propagates faster through the solid owing to larger material thermal conductivity as compared to gas medium, leading to more uniform heat transfer through the solid. By contrast, in the cavities, the convective flows are generated as a result of the temperature gradient-induced variations in gas density, as demonstrated in Fig. 1b. In consequence, thermal convection in cavities slows down heat transfer by conduction through the medium. The issue of energy transfer in the granular medium becomes far more complex for a reactive case, when additional intense mass exchange phenomena related to devolatilization, evaporation and chemical reactions, affecting the fluid flow dynamics come into play. Relaxation time as the resultant of these coupled effects depends on the particle diameter, bed porosity and heating rate.

## 2.1. Thermal wave propagation

The analysis of thermal wave propagation may be reduced to the solution of the energy balance problem while taking into account the equation for the heat flux of relaxation type (Eq. (1)).

In a one-dimensional case, assuming there is no macroscopic gas movement (i.e., for a porous bed with closed pores), the problem reduces to a system of equations:

$$\begin{cases} \rho c \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} = 0 \\ \theta \frac{\partial q}{\partial t} + \lambda \frac{\partial T}{\partial x} = -q \end{cases}, \quad (2)$$

where  $\rho$  and  $c$  denote material density and specific heat, respectively. This system of equations for a given vector of unknowns

$$\mathbf{y} = \begin{bmatrix} T \\ q \end{bmatrix} \quad (3)$$

may be represented in matrix form [19]

$$\mathbf{A} \frac{\partial \mathbf{y}}{\partial t} + \mathbf{B} \frac{\partial \mathbf{y}}{\partial x} = \mathbf{c}, \quad (4)$$

where

$$\mathbf{A} = \begin{bmatrix} \rho c & 0 \\ 0 & \theta \end{bmatrix}, \mathbf{B} = \begin{bmatrix} 0 & 1 \\ \lambda & 0 \end{bmatrix}, \mathbf{c} = \begin{bmatrix} 0 \\ -q \end{bmatrix}.$$

Considering the source-free conditions, the analysis of the problem given by Eqs. (3) and (4), and using the method of characteristics, one may arrive at the solution given as

$$\begin{cases} \frac{dw^{(1)}}{dt} = 0 & \text{if } \frac{dx}{dt} = \xi \\ \frac{dw^{(2)}}{dt} = 0 & \text{if } \frac{dx}{dt} = -\xi \end{cases}, \quad (5)$$

where the variables  $w^{(1)}$  and  $w^{(2)}$  are defined as

$$\delta w^{(1)} = \delta T + \sqrt{\frac{\theta}{\rho c \lambda}} \delta q, \quad (6)$$

$$\delta w^{(2)} = \delta T - \sqrt{\frac{\theta}{\rho c \lambda}} \delta q. \quad (7)$$

Parameter  $\xi$  in Eq. (5) represents the temperature signal propagation speed, which is dependent on the thermo-physical properties of a medium and the relaxation time, and is expressed as:

$$\xi = \sqrt{\frac{\lambda}{\rho c \theta}}. \quad (8)$$

One should note that in the case of non-homogeneous media, parameter  $\lambda$  is an effective quantity ( $\lambda = \lambda_{ef}$ ) that accounts for all mechanisms of heat transfer. The signal propagation speed is therefore influenced by the structure of the packed bed, such as the packing density, additionally affecting the fluid flow characteristics. It is thus related to the thermochemical process type. For instance, measurements regarding large-scale coal carbonisation report the temperature front to propagate through the packed coal layer with the speed of the order of  $10^{-6}$  m/s during the main process stage, which further increases up to the order

of  $10^{-4}$  m/s at the end stage owing to largely increased post-devolatilization bed porosity [22,23]. Experimental studies on the combustion of biomass reveal that the propagation speed of the burning front through such beds may vary between  $\sim 1 \times 10^{-4}$  m/s and  $5 \times 10^{-4}$  m/s, depending on the single particle combustion characteristics and bed density [24].

## 2.2. Integrated model of transport phenomena in a reactive granular bed

The one-dimensional numerical model, developed to simulate the thermal decomposition process of a packed bed of fuel particles was utilised to study the impact of relaxation time and physical parameters of the bed on the predicted dynamics of heat propagation. This model was previously used for simulating the real-scale coal coking process ([22]) and showed good agreement between the predictions and experimental data in terms of the total duration time of fuel decomposition. However, a discrepancy was observed in the temperature profile representing the moisture evaporation stage, which was considered to be due mostly to the simplified model of drying implemented. Having regard to the multiparameter impacts, the focus in the present work is on the effect of the key properties of a packed bed, such as moisture content and porosity, on the thermal wave propagation speed.

The process to be considered involves the packed bed drying and devolatilization stages. The proposed model is composed of balance equations, including mass balance for (i) solid and (ii) moisture released from the fuel, (iii) mass transport for gas mixture, (iv) momentum balance equation for gas mixture, (v) energy balance equation with convection term for packed bed, given as, respectively [22]:

$$\frac{\partial(\varepsilon_s \rho_s)}{\partial t} = -\dot{W}_{sg}, \quad (9)$$

$$\frac{\partial(\varepsilon_w \rho_w)}{\partial t} = -\dot{W}_{wg}, \quad (10)$$

$$\frac{\partial(\varepsilon_g \rho_g v_g)}{\partial x} = \dot{W}_{sg} + \dot{W}_{wg}, \quad (11)$$

$$\frac{\partial(\varepsilon_g \rho_g v_g v_g)}{\partial x} = -\frac{\partial(\varepsilon_g p)}{\partial x} - \frac{\varepsilon_g \mu v_g}{K}, \quad (12)$$

$$\frac{\partial(\rho c T)}{\partial t} + \frac{\partial(\varepsilon_g \rho_g v_g T)}{\partial x} = -\frac{\partial q}{\partial x} - \dot{W}_{sg} h_{sg} - \dot{W}_{wg} h_{wg}. \quad (13)$$

wherein the heat flux is described by the relaxation-type equation

$$q + \theta \frac{\partial q}{\partial t} = -\lambda_{ef} \frac{\partial T}{\partial x}. \quad (14)$$

Parameter  $\varepsilon$  in Eqs. (9) – (13) represents the volume fraction of the component (phase), and subscripts  $s$ ,  $w$ ,  $g$  refer to solid, water, and gas, respectively. Source term  $\dot{W}_{sg}$  stands for the mass release rate due to thermal decomposition (devolatilization) and is described through Arrhenius law, whereas  $\dot{W}_{wg}$  denotes the evaporation rate that is defined using a simplified approach [25], and  $p$  is the pressure. Quantities  $\mu$  and  $K$  stand for fluid viscosity

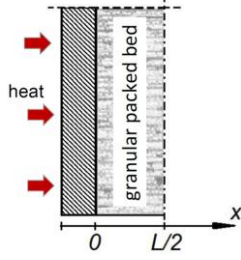


Fig. 2. A schematic representation of the considered one-dimensional problem of transport processes in reactive granular packed bed;  $L$  – total width of the bed layer.

and packed bed permeability. The bed is assumed to be isotropic, wherein the properties are averaged in the control volume. Thermo-physical properties of the packed fuel bed, i.e. density ( $\rho$ ), specific heat ( $c$ ) and thermal conductivity ( $\lambda_{ef}$ ) are the effective properties resulting from the fractions of solid, gas, and moisture. In addition, as regards the thermal conductivity, both, conduction ( $\lambda_c$ ) and radiation through the bed voids ( $\lambda_r$ ), were taken into account [22]. For the purpose of the analysis, the data of air were adopted for the gas mixture. The properties of gas and solid are summarised in Table 1.

The case of a layer ( $L$ ) of granular packed bed heated on both sides is considered. Assuming the process to be symmetric, the simulations were performed for the half-width of the considered packed bed, i.e. the calculation domain was  $0 \leq x \leq L/2$  (Fig. 2). The initial conditions were as follows:

$$T(x, 0) = T_0, \quad (15)$$

$$p(x, 0) = p_0, \quad (16)$$

$$v_g(x, 0) = 0, \quad (17)$$

$$\varepsilon_s(x, 0) = \varepsilon_{s,0}, \quad (18)$$

$$\varepsilon_w(x, 0) = \varepsilon_{w,0}. \quad (19)$$

The assumed boundary conditions include the values for temperature, evolved gas velocity and pressure, respectively:

$$T(0, t) = f(t), \quad \left. \frac{\partial T}{\partial x} \right|_{(L/2, t)} = 0, \quad (20)$$

$$v_g(0, t) = 0, \quad \left. \frac{\partial v_g}{\partial x} \right|_{(L/2, t)} = 0, \quad (21)$$

$$p(L/2, t) = p_0. \quad (22)$$

Function  $f(t)$  in boundary conditions (Eq. (20)) represent the time-varying temperature at  $x = 0$ , adopted from measurements [22,23].

The problem was solved partly implicitly. The mass and momentum equations were solved using explicit schemes, while an unconditionally stable implicit Crank-Nicolson algorithm was used to solve the energy equation. Further details of the model, including the numerical schemes used, can be found in the previous work [22].

Table 1. Thermo-physical properties adopted for simulation.

Parameter	Value	Ref.
$\varepsilon_{s,0}$	0.55	
$\rho_s$ [kg/m <sup>3</sup> ]	$\rho_s = \rho_s(T)$	[26]
$c_s$ [J/(kg K)]	$c_s = c_s(T)$	[27]
$\rho_g$ [kg/m <sup>3</sup> ]	(air, approximation of tabulated data) $\rho_g = \rho_g(T)$	[22]
$c_g$ [J/(kg K)]	$c_g = c_g(T)$	
$\mu_g$ [Pa s]	$\mu_g = \mu_g(T)$	
$\lambda_g$ [W/(m K)]	$\lambda_g = \lambda_g(T)$	
$K$ [m <sup>2</sup> ]	$5.0 \times 10^{-11}$	
$\lambda_{ef}$ [W/(m K)]	$\lambda_{ef} = \lambda_{ef}(T) = \lambda_c(T) + \lambda_r(T)$ , $\lambda_c(T) = 0.0031 \exp(0.063T) +$ $+ \varepsilon_w \rho_w$ , $\lambda_r(T) = 4\sigma ReT^3$	[22], [26], [28]
$\rho_w$ [kg/m <sup>3</sup> ]	1000.0	
$c_w$ [J/(kg K)]	4200.0	
$h_{wg}$ [J/kg]	$2200.0 \times 10^3$	
$h_{sg}$ [J/kg]	$200.0 \times 10^3$	[29]

### 3. Results and discussion

The variant simulations were performed to demonstrate the effect of packed bed properties, such as initial moisture content and porosity on the nature of solution and thermal front propagation speed, depending on the assumed relaxation time. Following previous studies [22], the relaxation time of 900 s was adopted as the maximum value considered. Furthermore, it shall be noted that simulation results regarding thermal behaviour of a spherical porous fuel particle undergoing decomposition in a hot gas stream indicate its heating times to be of the order of tens of seconds [12]. The mentioned study revealed that the outflow of released moisture and gas from the grain interior greatly contributes to slowing down the dynamics of its heating and decomposition. The characteristic process times for less porous particles are longer due to higher flow resistance. For instance, in the case of a 3 mm wet coal particle with a uniform thermal boundary condition at its surface and the intraparticle gas convection accounted for, the predicted heating time is around 60 s, whereas in the case of the same size wet biomass particle (far more porous) it is more than twice as short (~26 s). One may expect these times to be larger when considering the three-dimensional nature of transport processes and associated non-uniform particle surface heating in a granular packed bed.

In Fig. 3 the time-varying temperature evolution in reactive moist granular bed ( $\varepsilon_w=0.08$ , Fig. 3a) is compared with that for dry granular bed (Fig. 3b). In both bed cases, two significantly

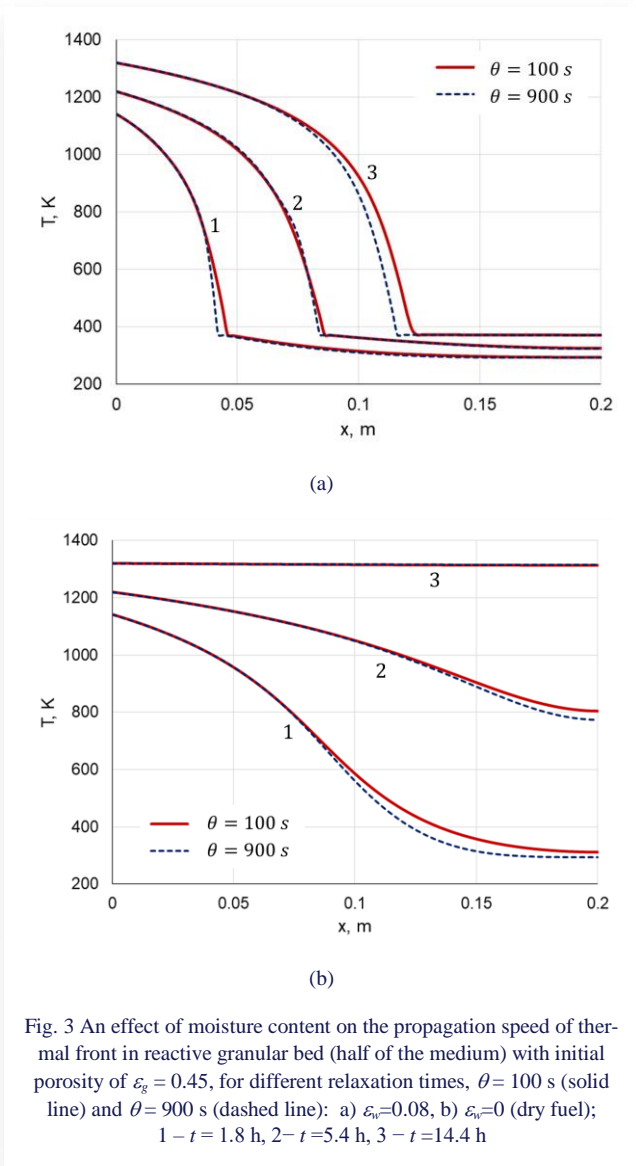


Fig. 3 An effect of moisture content on the propagation speed of thermal front in reactive granular bed (half of the medium) with initial porosity of  $\epsilon_g = 0.45$ , for different relaxation times,  $\theta = 100$  s (solid line) and  $\theta = 900$  s (dashed line): a)  $\epsilon_w = 0.08$ , b)  $\epsilon_w = 0$  (dry fuel); 1 -  $t = 1.8$  h, 2 -  $t = 5.4$  h, 3 -  $t = 14.4$  h

different relaxation times are taken into account, i.e.  $\theta = 100$  s and  $\theta = 900$  s. The simulation results show similar trends for both packed beds as regards the effect of relaxation time. Namely, for lower relaxation time the thermal front propagates through the granular medium faster than for the larger one. As expected, however, a considerable difference is observed in heating dynamics between wet and dry medium. In the case of a moist bed, there is a delay pronounced in the temperature increase above 373 K that is due to the thermal energy consumption for moisture evaporation. Unlike for the dry bed case, the results demonstrate a thermal front clearly separating the heated medium part from the cooler one. In other words, for the wet medium, the temperature gradients ( $dT/dx$ ) are larger. As a consequence, the difference between temperatures predicted for different relaxation times may reach hundreds of degrees. This may be seen in the case of simulated temperature curves for the process duration time of 14.4 hours (curves marked with 3, Fig. 3a), wherein the difference between predictions obtained for considered relaxation times at the distance of approx.  $x = 0.12$  m from the heated boundary ( $x = 0$ ) exceeds 200 degrees. For the dry

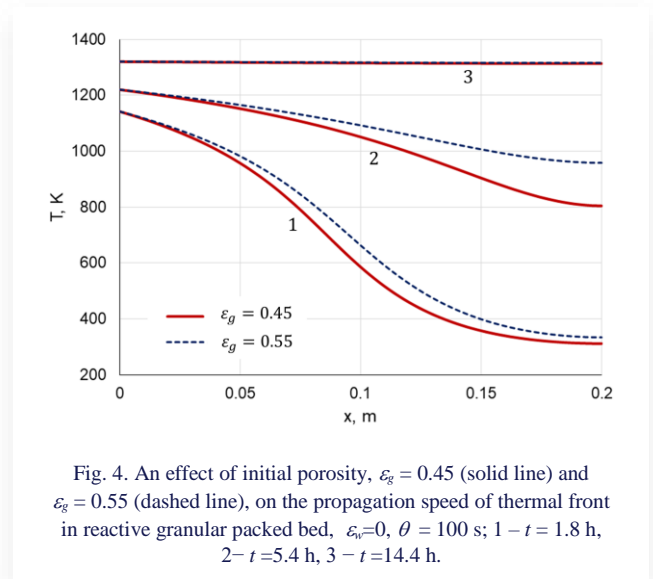


Fig. 4. An effect of initial porosity,  $\epsilon_g = 0.45$  (solid line) and  $\epsilon_g = 0.55$  (dashed line), on the propagation speed of thermal front in reactive granular packed bed,  $\epsilon_w = 0$ ,  $\theta = 100$  s; 1 -  $t = 1.8$  h, 2 -  $t = 5.4$  h, 3 -  $t = 14.4$  h.

bed case, characterized by a less sharp thermal front, these differences are far below 100 degrees, as displayed in Fig. 3b.

The model predictions indicated a quite significant impact of porosity (gas volume fraction) on the heat front propagation speed. The time-varying temperature distribution in dry packed granular bed ( $\epsilon_w = 0$ ) for different porosities, 0.45 and 0.55, and relaxation time of 100 s, are depicted in Fig. 4. As can be seen, heat propagates faster in the less dense packed bed, i.e. of larger porosity, owing to an increased contribution of radiation through the inter-particle voids. Furthermore, the differences in the temperature evolutions between granular beds differing in porosities increase with time, which clearly reveals the influence of variable structure-related bed properties. Nevertheless, these differences are smaller than those observed for temperature distributions, when water phase transition (moisture evaporation) comes into play, as shown in Fig. 3a (curves no. 3). The global effect of variable bed properties on the thermal wave propagation speed can be demonstrated by the analysis of a change in thermal diffusivity term ( $a = \lambda/(\rho c)$ ) during the process. Figure 5 presents the variation of thermal diffusivity in time along the

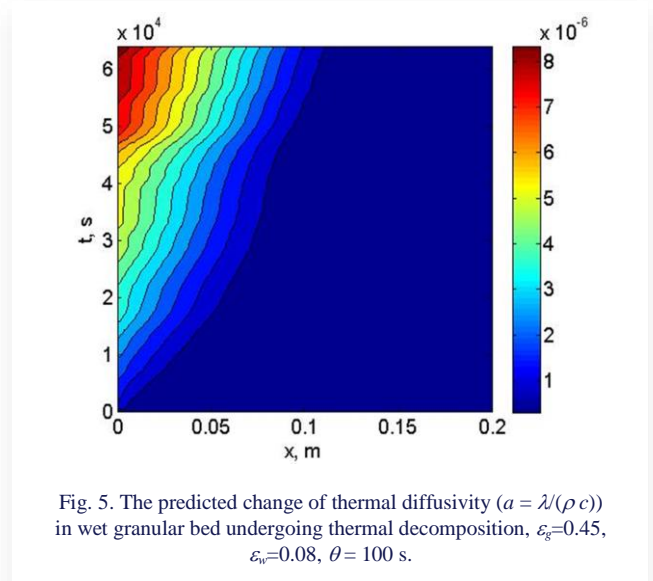


Fig. 5. The predicted change of thermal diffusivity ( $a = \lambda/(\rho c)$ ) in wet granular bed undergoing thermal decomposition,  $\epsilon_g = 0.45$ ,  $\epsilon_w = 0.08$ ,  $\theta = 100$  s.

packed bed layer of initial moisture content of 8% vol. and porosity of 0.45 during its thermal decomposition. As can be seen from the figure, the  $a$  value is below  $1 \times 10^{-6}$  m<sup>2</sup>/s in the cool unreacted part of a packed bed. As the process of decomposition proceeds, the thermal diffusivity increases by several times with the temperature rise and related change in the bed structure, reaching the value of over  $8 \times 10^{-6}$  m<sup>2</sup>/s at the end stage of the process. This corresponds with a nearly fivefold increase in the temperature signal propagation speed, i.e. from  $\sim 0.7 \times 10^{-5}$  to  $\sim 2.7 \times 10^{-5}$  m/s, respectively.

#### 4. Conclusions

In the paper, the non-classical approach was used to describe heat transfer in the reactive granular bed. Based on the predictions of the developed thermal and flow model that involves the relaxation-type (non-Fourier) heat conduction equation, the impact of the bed properties, including moisture content and porosity, on the thermal wave propagation speed through the medium was discussed. The simulation results served to indicate the role of a non-classical approach in the modelling of transport processes in reactive media of non-homogeneous inner structure. The obtained numerical results showed the dominant impact of moisture on slowing down heat propagation in the packed bed, leading to an increase in local temperature gradients.

The relaxation time accounted for in the developed one-dimensional model is a parameter that involves the coupled effects contributing to the change in energy flow direction in the interparticle voids, and thereby, to the delay in heat conduction in the medium. In this sense, the estimated value of relaxation time is affected by a degree of mathematical model simplification and, in particular, whether it accounts for the microscale effects of mass transfer. As regards the thermal processing of fuel particles, the precise determination of this characteristic time would require the detailed analysis of particle heating and devolatilization under a temperature gradient field. This would involve the use of mesoscale models enabling to map the interphase surface, as well as their experimental verification.

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