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A universal model of opposed flow combustion of solid fuel over an inert porous medium

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ABSTRACT

In this study, a universal model is developed to examine the behavior of combustion wave observed in porous solid matters (e.g., smoldering, self-propagating high-temperature synthesis (SHS), diesel particulate filter (DPF) regeneration process). Analytical expressions of the combustion characters of solid combustible (e.g., diesel particulate matters trapped in a DPF) deposited over an inert porous medium are obtained employing large activation energy asymptotic taking into account the sensible transport processes; namely, heat transfer between the porous medium and gas phases, radiation heat transfer from the porous medium, heat loss from the porous medium to the environment, mass transfer of oxygen from the gas stream to the surface of solid fuel and the effective diffusion in modeling the species diffusion. Then it has been validated that the present model is applicable and adaptable for predicting the characteristics of smoldering combustion and thus SHS process. As a result, the features of combustion wave of the present phenomena would be useful to other processes. From practical point of view and for deep understanding of the behavior of combustion wave of these processes, we investigate the effects of various physical parameters over a wide range of conditions. We observe that the moving speed of the reaction front increases with the increase of porosity of the porous medium, mass transfer coefficient and initial fuel mass fraction; while it decreases owing to the increase of heat transfer rate from the porous medium to the gas, heat loss to the environment and radiative heat transfer. Furthermore, the results reveal that extinction tends to occur due to lower porosity of the porous medium, higher radiative heat transfer from the porous medium, higher heat transfer rate from the porous medium to the gas and higher heat losses from the porous medium to the environment. Even the observed near-extinction behavior in reaction front speed versus heat loss diagram is found to be similar what we got in gaseous premixed flame propagating through the porous medium. An extinction limit diagram has been presented as a function of radiation-conduction parameter and the gas flow velocity. In addition to, the impact of radiation and the combined effect of the inclusion of Knudsen diffusion and tortuosity are demonstrated in terms of the spatial temperature and species profiles to examine how these two parameters modify the reaction front structure. Furthermore, the governing equations have been solved numerically and it is observed that asymptotic analysis gives a good agreement with the numerical solution.

1. Introduction

Smoldering is a slow, flameless and self-sustaining combustion wave which propagates through a porous fuel receiving most of the heat from heterogeneous oxidation of the fuel [1]. For propagation of the smolder wave, sufficient heat must be transferred from the exothermic reaction to the adjacent fresh fuel so that its temperature becomes high enough to initiate the oxidation of the fuel. Also enough oxygen must be present in the porous fuel, or infiltrated to the reaction zone from the surrounding to sustain the reaction. The same type of phenomena is observed in case of self-propagating high-temperature synthesis (SHS) and diesel particulate filter (DPF) regeneration processes. It should be noted that SHS and DPF regeneration are useful technological processes and the main demand in these processes is to control the propagation of the combustion wave without having extinction. On the other hand, in spite of being unwanted to several scientific disciplines, nowadays smoldering combustion is noticeably used for the development of new environmental and energy technologies [2]. Because the fundamental mechanisms of these processes are believed to be identical; the same mathematical model should be applied to illustrate these applications [3,4]. We observe that in some applications, reaction happens with the active participation of the porous medium, while in other cases reaction occurs in inert porous

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medium. Due to these two different types of contributions of the porous medium, the models developed to date in the field of smoldering combustion cannot be used effectively in other processes and vice versa. Hence, the formulation of a universal model has become inevitable so that it can be applicable for all of the above mentioned processes.

Now it is required to have knowledge about the important mechanisms of smoldering combustion, DPF regeneration process and SHS with a view to formulating a model. As research works based on modeling of these processes are rich enough, we will briefly review the modeling works on these processes and try to identify the key mechanisms that must be considered into a model.

1.1. Brief review of the past modeling works for smoldering combustion, DPF regeneration process and SHS

1.1.1. Transport mechanisms in modeling smoldering combustion

To identify the significant mechanisms of the propagation of the reaction front of smoldering combustion, a lot of theoretical and numerical models have been developed. Ohlemiller et al. [5] presented a detailed numerical model of reverse smolder combustion to provide useful insights of the controlling phenomena of the process. Analytical models [6,7] for forced cocurrent and opposed smoldering combustion, respectively, have been investigated in terms of the propagation velocity and flame temperature with the variation of physical parameters. They observed that extinction is occurred when all of the energy released in the reaction zone is used to heat the incoming gas. The above studies presumed the thermal and chemical equilibrium between the solid and gas phases based on the assumption that the contact time between them is extremely high. On the contrary, when the residence time of contact between the moving gas and the solid becomes short for thermal equilibration; the assumption of local thermal equilibrium between the phases is inappropriate [8]. Leach et al. [9,10] observed by the numerical simulation that the volumetric heat transfer coefficient, introduced to measure the intensity of the thermal nonequilibrium between the phases, demonstrates a significant impact on smolder velocity and even extinction is experienced owing to the high value of it. However, there is no theoretical works that could confirm this finding.

Not only the heat transfer between solid and flowing gas, other heat transfer processes are also necessary to consider for better prediction of propagation and extinction features in the present system. In fact, smolder wave propagates supported by heat released from the exothermic reaction. This heat released in the reaction zone is transferred not only to the gas but also toward the un-reacted material by conduction and radiation; and at the same time it is partially lost to the environment. Dosanjh et al. [6] and Leach et al. [10,11] observed that the radiative heat transfer significantly affects the reaction front structure and it becomes strong when pore diameters are large. Moreover, Leach et al. [10,11] solved their problems numerically taking only with and without radiation effect, regardless of changing the intensity of radiative heat transfer; while Dosanjh et al. [6] investigated just for two limiting values. Thus, for predicting the influence of radiation over a wide range of conditions, further study is required. Now, as mentioned above that heat is lost from the reaction zone to the surrounding environment. It has a large effect on the propagation of the reaction front and even it can cause extinction or quenching of the reaction front [1,6]. Nevertheless, any of the studies of Leach et al. [9–11] did not take into account the heat loss to the surrounding environment. In this regard, Rein et al. [12] extended the model of Leach et al. [11] including the heat losses to the surrounding environment. In a recent study, Rein et al. [13] proposed a novel model for both forward and opposed smoldering combustion. But they eventually neglected the chemical nonequilibrium effect in this model. Similar to other works of smoldering combustion, the models developed by Rein et al. [12,13] are only for the combustion of polyurethane foam. In addition to, their target was for better understanding of the controlling mechanisms of smolder combustion for the purpose of fire safety, yet they presented only the effect of inlet gas velocity over a range for microgravity. Furthermore, the models are solved numerically which is generally difficult to carry out for anybody to investigate the effects of other physical parameters. So, this demands further study with a model that includes the heat loss to the environment. As heat transfer from the solid to the gas is important when thermal nonequilibrium exists between the phases, mass transfer from the gas stream to the surface of fuel is also essential in case of chemical nonequilibrium between the phases. Although one should not straightforwardly take the chemical equilibrium between the phases without being certain of its validity [4], most of the theoretical studies published to date ignored the chemical nonequilibrium due to the complexity of the model or presuming the chemical equilibrium between the phases. The effect of the chemical nonequilibrium is considered in [9,11–14] through the mass transfer coefficient. But it has not been investigated in any of these studies except Wang et al. [14]. They found that the smolder propagation velocity increases with the increase of the mass transfer coefficient. It is noted that one feature that is generally ignored in traditional modeling approaches in modeling the species diffusion through the porous medium is the effective diffusivity. Regarding the importance of effective diffusivity in smoldering combustion, Ohlemiller [1] used the more conventional approach for the effective diffusivity due to the lack of evidence on the pore structure developed in smoldering and emphasized that a better description has to be used. It has been ignored taking the highly porous medium so that oxygen diffusion is independent of porosity. Thus, the scope of using an advanced definition of effective diffusivity remains untouched in the field of smoldering combustion.

From the above discussion we can come to the conclusion that the essential mechanisms in smoldering combustion are heat transfer from the solid to the gas, radiative heat transfer, heat loss to the environment, mass transfer from the bulk gas to the surface of fuel and effective diffusivity.

1.1.2. Transport mechanisms in modeling DPF regeneration process

Under the framework of finding the important mechanisms of smoldering, DPF regeneration process and SHS, we will now review the modeling works on DPF regeneration process. Mathematical modeling is commonly used for the better understanding of the process and thereby for development of system optimization. Pioneer works in modeling the thermal regeneration of a wall-flow monolith DPF are [15–17] which have been developed presuming only the thermal nonequilibrium between the solid and the exhaust gas temperature. The chemical nonequilibrium and heat loss from the solid phase are neglected. But in recent years chemical nonequilibrium between the solid and gas phases [18–20] and both the thermal and chemical nonequilibrium between them [21–24] are taken into account in the models. The effect of heat transfer coefficient related to the thermal nonequilibrium has been investigated by Flytzani-Stephanopoulos et al. [25]. They observed that the large value of heat transfer coefficient reduces the heat conduction through the solid resulting in lower DPF temperature. During the regeneration process the DPF temperature becomes high, so the radiative heat transfer could have significant effect. Haralampous and Koltsakis [26] and Dardiotis et al. [21] developed models incorporating the radiative heat transfer along with the thermal and chemical nonequilibrium. Koltsakis and Stamatelos [27] formulated a model considering only the thermal and chemical nonequilibrium between the phases while Depcik and Assanis [24] presented a variety of models including not only the thermal