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An attempt to close the recycling loop**

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Publication date

2017

Document Version

Final published version

Published in

HISER International Conference

Citation (APA)

Teklay, A., Vahidi, A., Lotfi, S., Di Maio, F., & Rem, P. (2017). Numerical modelling of the dehydration of waste concrete fines: An attempt to close the recycling loop. In F. Di Maio, S. Lotfi, M. Bakker, M. Hu, & A. Vahidi (Eds.), *HISER International Conference: Advances in Recycling and Management of Construction and Demolition Waste, 21-23 June, Delft, The Netherlands* (pp. 18-24). Delft University of Technology.

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Numerical modelling of the dehydration of waste concrete fines: An attempt to close the recycling loop

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Abstract

The ever-increasing interest on sustainable raw materials has urged the quest for recycled materials that can be used as a partial or total replacement of fine fractions in the production of concrete. This paper demonstrates a modelling study of recycled concrete waste fines and the possibility of turning them into active constituents for the production of concrete. When construction demolition waste (CDW) fines with particle size 0 - 4mm are exposed to a hot environment, different reactions will occur, especially dehydration and phase changes. A one-dimensional (1D) transient model is developed to predict the conversion of the hydrated concrete fines into their dehydrated state, in which the key processes inside the particle and at the boundary layer outside the particle are properly addressed. The model predicts a final composition of the particle that resembles cement clinker, which means a high potential for reuse in manufacturing concrete. Finally, model results for the mass loss during conversion are experimentally validated using thermogravimetric study.

Introduction

The quantities of construction and demolition wastes (CDW) have been increasing significantly in the last decade and the trend is even expected to rise progressively for the decade ahead. Hence, a sustainable way of managing CDW is mandatory in order to abate the problems associated with waste disposal and resource utilization. There have been a number of attempts to recycle construction demolition wastes and specifically concrete [1]. So far, the coarser fractions have been successfully recycled and implemented into new concrete mixes and road bases. However, there is only little effort to recycle the CDW fine fractions (0- 4mm) and this part of research is lagging compared to its corresponding coarse fraction. The use of fine recycled materials in the construction industry is seldom practised and the CDW fines usually end up in a landfill. Due to the serious environmental problems posed by the dumping of construction demolition wastes and the potential of producing low-CO₂ Calciumsilicates, it is necessary to look for ways of recovering the important minerals out of the construction demolition wastes.

Unlike most research articles, where thermal decomposition of concrete has been studied to examine the property of concrete during fire[2][3][4] , this article prompts the attention and the possibility of reusing End of life (EoL) concrete wastes after being activated through thermal treatment.

Shui et al. reported on the potential use of CDW fines for further use in the concrete industry and their potential to be rehydrated to form cement paste [5]. Accordingly, when a hydrated cement paste is exposed to different temperatures ranging 300-900 °C, it loses most of the free and bound water. When rehydrated again, positive results such as quick setting time, rapid rehydration rates and reasonable compressive strength were noticed [5].

The most common effort to recycle the fine fraction of CDW is to use thermal energy and comminution[6]. This helps to activate the fine fraction by getting rid of the bound water embedded in hydration products of concrete.

This paper presents a 1D modelling effort to fully address the detailed phenomena that occurs when CDW fines are exposed to high temperatures. The particle model assumes a spherically shaped particle and this particle is discretised into a number of spherically shaped concentric circles (control volumes) where the momentum, energy and species transport equations are numerically solved at each control volume by using a finite volume method [7] [8].

Mathematical modelling

When fine particles from concrete demolition wastes are exposed to a hot environment, they will undergo a series of reactions, including dehydration, dehydroxylation, phase transformation and decarbonation. The reactions considered in this study are summarized in Table 1:

Reaction	E [kJ/mol]	A [s ⁻¹]	Reference
H ₂ O (l) ⇌ H ₂ O (g)	88	5.13e+10	[9]
Ca(OH) ₂ ⇌ CaO + H ₂ O(g)	151.82	6.566e+7	[10]
(CaO) _a SiO ₂ (H ₂ O) _b ⇌ (CaO) _a SiO ₂ (H ₂ O) _{b-c} + c.H ₂ O(g)	225	4.85e+8	[10]
CaCO ₃ ⇌ CaO + CO ₂ (g)	160	2.91e+7	[11]
SiO ₂ (α) ⇌ SiO ₂ (β)	274	1.75e+10	[12]

Table 1. Chemical reactions included in the model and their respective kinetic parameters (E , Activation energy and A , frequency factor).

Integration in time proceeds by updating particle property at a new time $t + \Delta t$ from initial parameters at time t . The model involves the calculation of coupled partial differential equations of energy and species transport to obtain detailed profiles of temperature, particle composition and other properties. The equations that govern the heat and mass transfer with in the particle and its surrounding are:

$$\left\{ \begin{array}{l} \frac{\partial(\varepsilon \rho_g)}{\partial t} + \text{div}(\varepsilon \rho_g \vec{u}) = S_g \\ \vec{u} = -\frac{\eta}{\mu} \frac{\partial P}{\partial r} \\ \frac{\partial}{\partial t} \left(\sum_{\text{solid},i} \rho_i h_i + \sum_{\text{liquid},k} \rho_k h_k + \varepsilon \rho_g h \right) + \text{div}(\varepsilon \rho_g \vec{u} h) = \text{div}(k_{\text{eff}} \nabla T) + \text{div}(-\sum_j h_j \vec{J}_j) + S_h \\ \frac{\partial(\varepsilon \rho_g Y_j)}{\partial t} + \text{div}(\varepsilon \rho_g \vec{u} Y_j) = \text{div}(-\vec{J}_j) + S_{Y_j} \end{array} \right. \quad (1)$$

where ε , ρ_g , t , \vec{u} , S_g , η , μ , P , r , h , k_{eff} , T , \vec{J}_j , S_h , Y_j and S_{Y_j} represent the porosity, gas density, time, gas velocity, source term in gas mass conservation equation, permeability, gas dynamic viscosity, pressure, radius, sensible enthalpy, effective heat conductivity, temperature, diffusion flux of gas species in the gas mixture, source term to the energy equation, mass fraction of gas species j , and source term to j^{th} gas species transport equation, respectively.

The boundary conditions at the particle surface are evaluated based on reference conditions which are approximated based on averaging calculations [13] and hence all properties at the particle boundary are calculated based on these parameters. The heat and mass transfer coefficients (h_T and h_m , respectively) between the particle surface and its boundary surrounding are evaluated from Nusselt number (Nu) and Sherwood number (Sh) [14]. For spherical particles, the empirical correlations of heat and mass transfer coefficients are calculated as:

$$\begin{cases} \text{Nu} \equiv h_T d_p / k_g = 2 + 0.64 \text{Re}^{1/2} \text{Pr}^{1/3} \\ \text{Sh} \equiv h_m d_p / D_{AB} = 2 + 0.64 \text{Re}^{1/2} \text{Sc}^{1/3} \end{cases} \quad (2)$$

Where d_p , k_g , D_{AB} , Pr and Sc are the particle diameter, gas conductivity, molecular diffusivity, Prandtl number and Schmidt number. The Reynolds number, Re is calculated based on the freestream density, ρ_∞ and the viscosity, μ in the boundary layer [$Re = \rho_\infty |u_\infty - u_p| d_p / \mu$], as it is the ratio of inertia to viscous forces. The source term on mass conservation equation of gaseous species is based on the generation of gaseous species due to the rate of reaction from Arrhenius' equation where $rate = A_i \exp(-E_i/RT) \rho_i$, where A_i , E_i , T and ρ_i are the pre-exponential factor, the activation energy, temperature and the density of the consequent species, respectively.

Numerical method

The particle geometry is divided into a number of spherical shells (or cells) in the radial direction. The governing equations shown above (Eq. 1) are discretized using the finite volume method. For all the transport equations, the fully implicit scheme is used for transient terms. The upwind scheme is applied for the convection term, and the central difference scheme is employed for the diffusion term. A staggered grid is used for velocity components. The grid-independence of the solution has been tested to secure sound numerical results. Accordingly, for the 1D model of a 1mm diameter spherical particle, the particle is divided into 40 concentric spherical shells and a time step size of 1 ms is used in the transient modelling. All the above processes are numerically implemented into C++ code and solved using Tridiagonal Matrix Algorithm (TDMA) solver.

Experimental study

Thermogravimetric analysis was carried out using NETZSCH simultaneous thermal analyser TG-449-F3-Jupiter under controlled atmosphere. In our case Argon gas was used. About 32.4 mg of CDW fines (with particle size < 0.1 mm) was placed on a Pt crucible. The sample was heated to a maximum temperature of 1000 °C at a heating rate of 10 °C per minute. The mass loss history conveyed from the TGA study is used to validate the model results.

Result and Discussion

The transient 1D model predictions and final results are based on the initial composition and assumptions of the concrete fine fractions. For instance, the porosity and the permeability of the model is assumed constant, the spherical concrete fines are represented by a spherical shaped particle of 1mm in diameter which has the initial composition of 10% moisture, 15%

Ca(OH)_2 , 35% of SiO_2 , 40% CSH and 10% CaCO_3 . When such a particle is exposed to a hot surrounding at 1000 °C, the particle surface is the first to get the influence of heating. The heat and mass transfer is therefore commenced by convection and radiation. As it reaches the surface, the heat transfer is ruled by conduction. The mass transport due to evolution of gases is through diffusion. Figure 1 depicts the temperature profile of the particle, showing that the particle surface experiences a higher temperature than the particle core until the particle becomes isothermal at equilibrium. The observed differences in temperature between the particle surface and particle core at the earlier time is due to the outward diffusion of water that impedes the inward movement of heat. Eventually the particle becomes isothermal after 16 seconds.

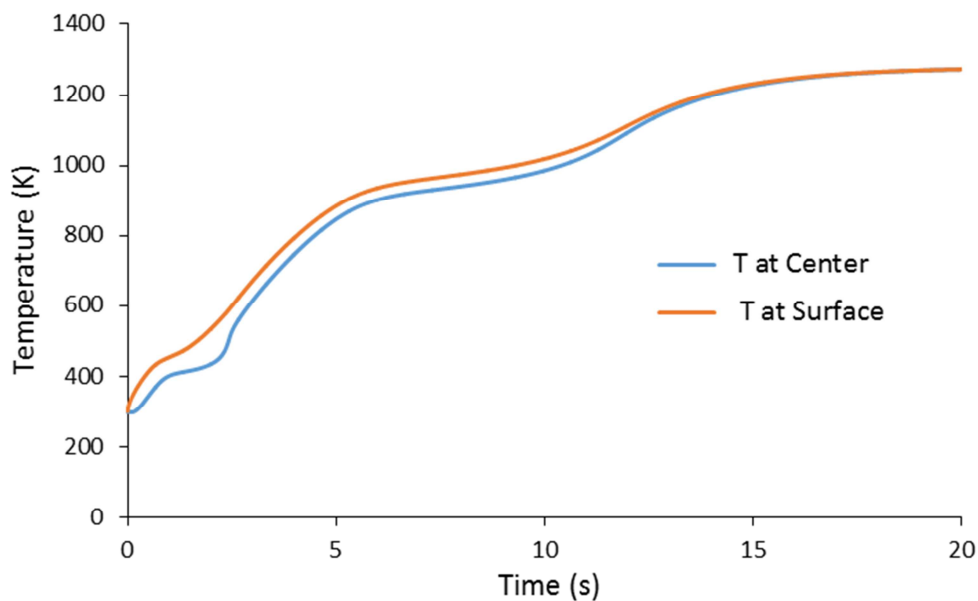


Figure 1. The evolution of temperature at particle surface and particle centre.

Once the advancement of particle temperature from the surrounding to the entire particle is implemented, the reactions described in Table 1 will commence as the particle temperature rises. Accordingly, dehydration, dehydroxylation, phase transformation and decarbonation reactions will continue. The extent of consumption of solid species and generation of gaseous species (new solid species) depends on the activation energy and frequency factor of each reaction. Therefore, the consumption of Portlandite and limestone generates new species CaO and H_2O (g). CSH is decomposed into new species C_2S which is one of the active components that exist in Portland cement. $\alpha\text{-SiO}_2$ is transformed to $\beta\text{-SiO}_2$, but again transforms back to the $\alpha\text{-SiO}_2$ on cooling. Figure 2 explains the changes in composition of the construction demolition waste fines modelled based on the above case.

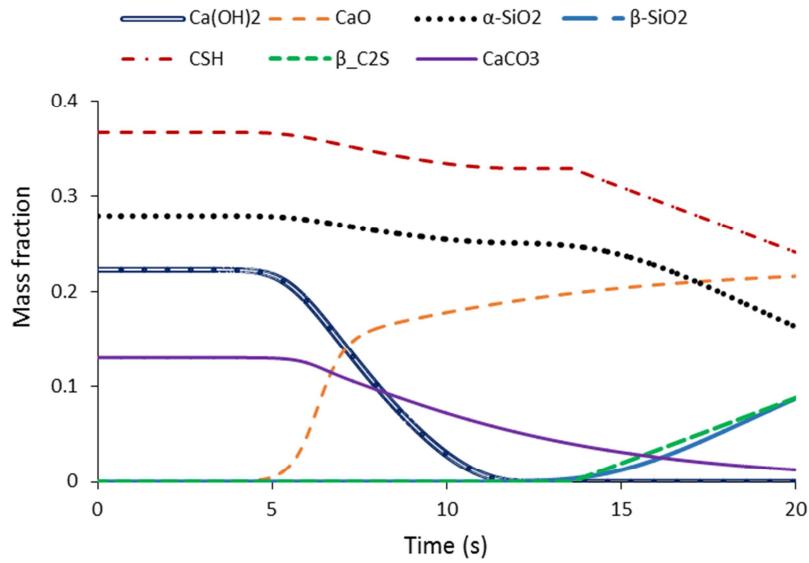


Figure 2. Changes in composition of solid species inside the particle model.

Since the ultimate objective of this study is to evaluate the final composition of the CDW fines after heat treatment and assess their suitability for recycling, the model prediction confirms the suitability of the final composition by correlating with the composition of cement clinker. Figure 3 shows the final composition of the particle model after being exposed to high temperature in terms of CaO, β-C₂S, SiO₂, CSH and CaCO₃. The presence of CSH in the final composition indicates the difficulty of removing the interstitial water molecules that makeup the CSH crystals [10]. Apart from CSH, the presence of all other components i.e. CaO, β-C₂S, SiO₂ and CaCO₃, shows the similarity of model composition with cement clinker. This assures the suitability of CDW fines for reuse in the production of concrete. The only source of CO₂ emission is due to decomposition of CaCO₃ which is really small in amount. Thus, one can easily realize the attempt to recycle concrete fines by thermal treatment is a green method. Process temperature can be controlled to tailor the desired products and of course to deal with the economics of recycling.

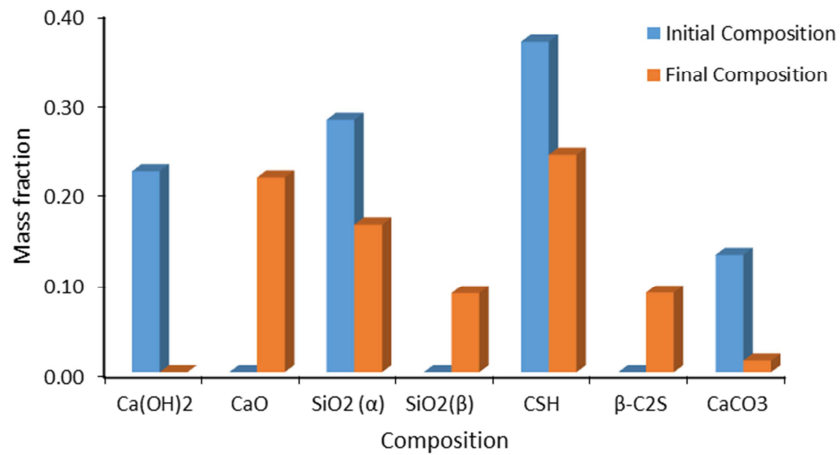


Figure 3. The final composition of CDW fines after exposed to 1000 °C for 20s.

Comparison between particle conversion profile of the model and mass loss experiments under thermogravimetric (TG) conditions is provided in Figure 4. The conversion in this context is based on the initial and final amount of water (*conversion*, $x = (m_i - m_t)/(m_i - m_f)$) where m_i , m_t and m_f are the initial mass of water, the mass of water at time t and final mass of water, respectively. In order to reasonably compare the model prediction with the experimentally recorded mass loss, the conditions in the model are appropriately adapted to mimic the heating rate and atmosphere of TGA. As such, radiation model is disabled in the model, the ambient gas velocity is set to a negligible value, and the ambient gas temperature is set as a linear function of the heating rate (10 °C/minute). As shown in Figure 4, the conversion profile recorded in TG analysis and the model prediction show acceptable agreement. Keeping in mind the differences in details of heat and mass transfer in the TGA environment and other uncertainties, the small discrepancy can be understood.

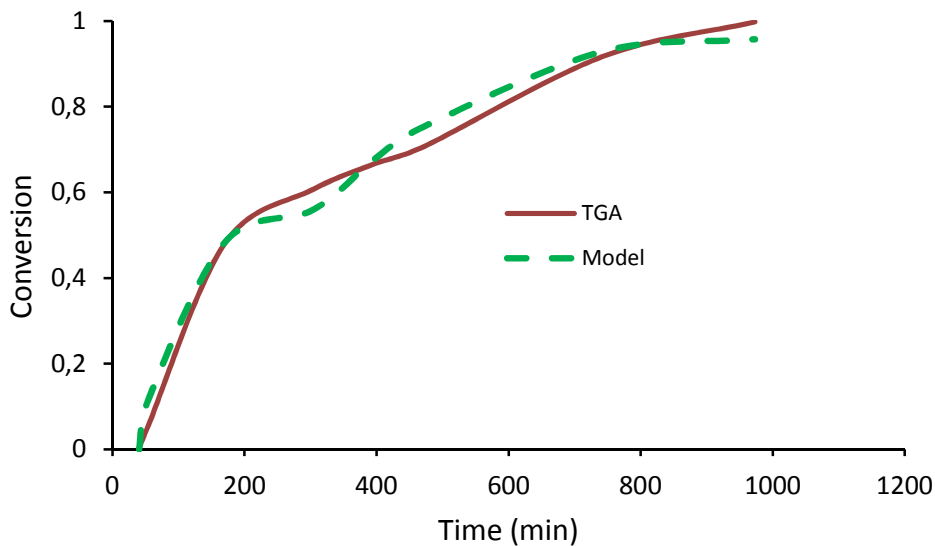


Figure 4. Validation of the conversion profile of model with scaled mass loss recorded in TGA (32.4 mg fines, 10 °C/min, and 1000 °C).

Conclusion

The dehydration of concrete fines has been studied numerically by developing a 1D transient model using C++ code. The model is capable of predicting the changes in composition when the fine fraction from construction demolition wastes are exposed to high temperature. Consequently, the final composition of the CDW fines show similar composition as that of cement clinker providing potential for reuse and for substituting cement partially or fully depending on the recipe of the target concrete.

The model can further predict the optimum process conditions that may help to convert the concrete waste fines into a reactive composition to reasonably address the cost and application balance of the recycled end product.

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