MULTIPHYSICS LATTICE DISCRETE PARTICLE MODEL FOR THE SIMULATION OF CONCRETE THERMAL SPALLING

LEI SHEN\(^*\), WEIXIN LI\(^†\), XINWEI ZHOU\(^‡\), JUN FENG\(^◦\), GIOVANNI DI LUZIO\(^*\), QINGWEN REN\(^⋄\), AND GIANLUCA CUSATIS\(^⋆\)

\(^*\)Hohai University, Nanjing, Jiangsu China
e-mail: shenlei-hhu@foxmail.com

\(^†\)Northwestern University, Evanston, IL USA
e-mail: lwx3000@gmail.com

\(^‡\)ES3, San Diago, CA USA
e-mail: xinwei.zhou@es3inc.com

\(^◦\)Nanjing University of Science and Technology, Nanjing, Jiangsu China
e-mail: fengjun2016@hotmail.com

\(^*\)Politecnico di Milano, Milan, Italy
e-mail: giovanni.diluzio@polimi.it

\(^⋄\)Hohai University, Nanjing, Jiangsu China
e-mail: renqw@hhu.edu.cn

\(^⋆\)Northwestern University, Evanston, IL USA
e-mail: g-cusatis@northwestern.edu

Key words: concrete thermal spalling, high temperature, discrete, lattice discrete particle model, hygro-thermal coupling

Abstract. Explosive thermal spalling behavior during fire exposure is one of the major issues in the design of modern reinforced concrete structures. However, spalling mechanisms and their interaction still remain in dispute in the scientific community. In order to shed some light on this phenomenon, a discrete hygro-thermal model of concrete at high temperature called DTemPor3 is proposed and a full coupling scheme between DTemPor3 and the Lattice Discrete Particle Model (LDPM) is adopted. The proposed multi-physical coupled model features the effect of pore pressure and temperature on the mechanical response as well as the impact of cracking on moisture mass transport and heat transfer. This proposed model can reproduce the explosive spalling phenomenon and only when the effect of thermal stresses is taken in account along with the effect of pore pressure on crack initiation, as demonstrated by the numerical simulations.

1 INTRODUCTION

Concrete tends to be very sensitive to explosive spalling when it is exposed to fire and its sensitivity to this phenomenon must be considered and controlled in the design and construction of reinforced concrete structures, especially for the design of tunnels. As a result, thermal spalling of concrete has been a hot topic for the scientific community over the last
30 years. However, the main driving mechanisms are not completely clear due to the complex interaction of heat transfer, moisture mass transport, as well as mechanical and chemical behavior of concrete at high temperature. On the one hand, the pressure builds up in the concrete pores as a consequence of the physically and chemically bound water in the cement that vaporizes at high temperature, and it leads to tensile stresses in the heated concrete [1]. On the other hand, the restrained thermal dilation generate a biaxial state of stress with compressive stresses parallel to the heated surface and tensile stresses perpendicular to the heated surface [2]. Internal stresses build up as a result of the combined effect of pore pressure increase, thermal stresses derived from temperature gradients, mismatch between the deformation of different constituents, and the shrinkage associated with water release [3,4]. When the internal stresses exceed the maximum tensile strength, cracks and/or spalling occur.

Although some reasonable discussions on the various mechanisms were given in previous studies [5–7], there were no evident results persuading other researchers because the dynamic explosive fragmentation due to the spalling phenomena was not simulated correctly by the traditional continuous finite element approaches. Therefore, this study responds to an actual need for a reliable computational tool capable of simulating the dynamic explosive fragmentation during spalling.

In this study, a discrete temperature and pore vapor pressure model in 3D (called DTemPor3) is formulated and implemented within the framework of the Lattice Discrete Particle Model [9]. The spalling phenomena observed in the experiments [12] are reproduced and the main driving mechanisms are discovered.

2 The Computational Framework
2.1 The Lattice Discrete Particle Model at high temperature

The Lattice Discrete Particle Model (LDPM), originally formulated by Cusatis et al. [9], is able to accurately capture the failure behavior of concrete at room temperature as demonstrated in many previous studies. This study proposes an improvement of LDPM in order to allow the simulation of concrete behavior at high temperature.

LDPM simulates the concrete mesostructure by taking into account the interaction of coarse aggregate pieces. Coarse aggregate pieces with different size are randomly placed inside the concrete volume following the Fuller sieve curve. A typical aggregate distribution is shown in Fig. 1(a) in 2D and (d) in 3D. The Delaunay tetrahedralization is used to connect the centers (termed “nodes”) of the spherical particles to produce tetrahedra. The edges of the tetrahedra form the lattice system that describes the interaction between adjacent particles as shown in Fig. 1(b) in 2D. A domain tessellation is performed to define a set of 12 potential failure locations (termed “facets”) in each tetrahedron (see in Fig. 1(f)). The tessellation procedure is described in detail in Cusatis et al. [9]. By connecting the facets surrounding each aggregate center, a system of polyhedral cells is obtained as illustrated in Fig. 1(c) in 2D and (e) in 3D.

The facet strains between two adjacent Tet-nodes are defined as $e = [e_N, e_M, e_L]^T$, where $e_N = n^T[u]/l$ is the normal strain component, $e_M = m^T[u]/l$ and $e_L = l^T[u]/l$ are the tangential strain components, $[u]$ is the displacement jump at the centroid of the facet, $l$ is the
tetrahedron edge associated with the facet and \( \mathbf{n}, \mathbf{m}, \) and \( \mathbf{l} \) are unit vectors normal and tangential to each facet. By assuming additivity of strains, one can write:

\[
\dot{\mathbf{e}} = \dot{\mathbf{e}}^s + \alpha_T \dot{T} \mathbf{n} \tag{1}
\]

in which \( \dot{\mathbf{e}}^s \) represents stress-related strains and the term \( \alpha_T \dot{T} \) represents the thermal expansion is the main impose normal strain, \( \dot{T} \) is the temperature rate and \( \alpha_T(T) \) is the thermal expansion coefficient which is an overall result of the cement shrinkage and aggregate dilatation occurring at high temperature [2].

The LDPM elastic behavior is described by assuming that the normal and shear tractions acting on the solid skeleton proportional to the corresponding strains. One can write \( \mathbf{t}^s = [t_N^s \, t_M^s \, t_L^s]^\top \), where \( t_N^s = E_N \varepsilon_N^s \) is the normal component, \( t_M^s = E_M \varepsilon_M^s \) and \( t_L^s = E_L \varepsilon_L^s \) are the shear components; \( E_N = E_0, \ E_M = \alpha E_0, \ E_0 \) is the effective normal elastic modulus estimated by Young’s modulus and Poisson’s ratio. \( \alpha = 0.25 \) is the shear-normal coupling parameter. The detail constitutive relations describing the inelastic behavior are formulated in Cusatis et al. [9].

The mesoscopic crack opening vector associated with each facet can be calculated as \( \delta = \delta_N \mathbf{n} + \delta_L \mathbf{l} + \delta_M \mathbf{m} \), where \( \delta_N = l (\varepsilon_N^s - t_N^s/E_N) \), \( \delta_L = l (\varepsilon_L^s - t_L^s/E_L) \), \( \delta_M = l (\varepsilon_M^s - t_M^s/E_M) \). \( \delta_N \) is its normal component, and \( \delta_M \) and \( \delta_L \) are two shear components related to the sliding of crack surfaces.

Thermal degradation in LDPM is introduced through the following function:

\[
f_d = 1 - \frac{\exp(n_d)\Theta}{1 - \Theta(1 - \exp(n_d))} \tag{2}
\]

where \( n_d \) is the parameter controlling the shape of the thermal degradation evolution and \( \Theta \) is a temperature level variable, \( \Theta = ( (T - T_s)/(T_m - T_s)) \), \( T_s \) is the temperature at which concrete starts to degrade and \( T_m \) is the temperature at which concrete starts to melt. LDPM material parameters, \( \sigma_t, \ \sigma_s, \ E_0, \ \sigma_c \) and \( \sigma_{N0} \) are assumed to decay proportional to \( f_d \) in

\begin{table}[h]
\centering
\begin{tabular}{lccc}
\hline
\textbf{Parameters} & \textbf{\( T_s \)} & \textbf{\( T_m \)} & \textbf{\( n_d \)} \\
\textbf{Unit} & [\degree C] & [\degree C] & [-] \\
\hline
\textbf{\( \sigma_t \)} & Tension strength & 274 & 1000 & 0.4 \\
\textbf{\( \sigma_s \)} & Compression strength & 274 & 1000 & 0.4 \\
\textbf{\( E_0 \)} & Effective normal elastic modulus & 20 & 1000 & 0.7 \\
\textbf{\( \sigma_c \)} & Compression yielding strength & 340 & 1000 & 0.2 \\
\textbf{\( \sigma_{N0} \)} & Transitional strength & 340 & 1000 & 0.2 \\
\hline
\end{tabular}
\caption{Thermal degradation of LDPM parameters}
\label{tab:thermal-degradation}
\end{table}

\[
\mathbf{t} = \mathbf{t}^s - b p \mathbf{n} \tag{3}
\]

where, \( p \) is pore pressure and \( b \) is the Biot coefficient [13, 14] which is assumed to be equal to 1 unless otherwise mentioned in the current formulation [5]. Finally, equilibrium equations are obtained through the force and moment equilibrium of each cell surrounded by a group of facets.

\section{2.2 The Hygro-Thermal model}

Considering the discrete character, the hygro-thermal equations are formulated with reference to a 3D network of 1D elements anchored to the LDPM geometry [14]. Let’s consider two Tet-points inside two adjacent LDPM tetrahedra labeled as node “T1” and “T2” in the 2D representation of Fig. 2 (a). The segment connecting T1 and T2 is called “Flow Lattice Element” (FLE) [2]. Each FLE has an associated volume, and the average of pore pressure
and temperature on “T1” and “T2” represent the mass thermodynamic state in the FLE12 domain volume. Accordingly, for each FLE, the mass and heat balance equations can be written as:

\[
\frac{d}{dt} (V_{e}w_{e} + V_{i}c_{i}) = A_{w} \left( D_{1}\frac{p_{i}-p_{f}}{l_{12}^{2}} + D_{2}\frac{f_{i}-f_{f}}{l_{12}^{2}} \right) \tag{4}
\]

\[
\frac{d}{dt} (V_{e}U_{e} + V_{i}U_{i}) = A_{w} \left( D_{1}\frac{p_{i}-p_{f}}{l_{12}^{2}} + D_{2}\frac{f_{i}-f_{f}}{l_{12}^{2}} \right) \tag{5}
\]

where, \( t \) is time; \( p_{i}(t) \) and \( T_{i}(t) \) are pore pressure and temperature at \( T_{i} \), \( i = 1, 2 \); \( V_{e} = \sum_{i=1}^{2} V_{ei} \) is the FLE12 domain volume; \( l_{12} = \sum_{i=1}^{2} l_{i} \) is the FLE12 length and the superscript \( i = 1, 2 \) identify variables relevant to the Side \( T_{1} \) and the Side \( T_{2} \), respectively. In Fig. 2 (b), \( a \) is the unit vector orthogonal to the tetrahedron face \( P_{1}P_{2}P_{3} \), and \( e \) is the direction of FLE12 from \( T_{2} \) to \( T_{1} \). The projection of the area \( P_{1}P_{2}P_{3} (A_{\Delta}) \) in the \( e \) direction is defined as \( A_{w} = -A_{\Delta}a^{T}e \). One can write \( V_{e} = l_{12}A_{w}/3 \) and the domain volume increase is assumed to come from the initiation and propagation of cracks on the corresponding facets \( (V_{e} = \sum_{i=1}^{2} \sum_{j=1}^{3} (\delta_{NP_{j}} A_{FP_{j}})) \) and the elastic volume increase of \( V_{ei} \) is neglected. \( \delta_{NP_{j}} \) denotes the normal crack opening of a facet connecting with \( T_{i} \) and \( A_{FP_{j}} \) is the corresponding facet area.

\[
V_{w}(T, p) \text{ gradually releases in the pores for temperatures ranging from } 105^\circ \text{C to } 1000^\circ \text{C. The empirical equation proposed by Gawin et al. } [7] \text{ is used as evolution law for this process. If } T \leq 105^\circ \text{C}, \ w_{d} = 0. \text{ Otherwise, when } T > 105^\circ \text{C, } w_{d} = 0.32\alpha_{c}^{\infty}c_{j}(T_{\text{max}}(t)), \text{ in which, } \alpha_{c}^{\infty} = 1.032w_{\text{mix}}/c/(0.194 + w_{\text{mix}}/c) \text{ is the asymptotic hydration degree } [15]; \ w_{\text{mix}} \text{ is the initial water in the concrete mix; } T_{\text{max}} \text{ is the highest temperature reached by concrete during heating; } f_{j}(T) \text{ is a dimensionless function of temperature which could be found in } [7].
\]

\[
U_{w}(p, T) \text{ denote the heat content per unit volume of uncracked material. It can be expressed as the algebraic sum of the heat density in the uncracked material and the heat consumption due to the dehydration. One can write as } U_{w} = U_{s} - U_{d}, \text{ where } U_{s} = \rho_{s}C_{s}T \text{ is the heat density in uncracked material with the solid skeleton density } \rho_{s} = 2400 \text{ kg/m}^3, \text{ and the heat capacity } C_{s} = 900 + 80(T_{C}/120) - 4(T_{C}/120)^{2} \text{ kg/m}^3/\text{K} \text{. The dehydration heat consumption is defined as } U_{d} = C_{d}w_{d}, \text{ in which } C_{d} = 2400 \text{ J/kg } \text{is the heat consumption of dehydration per kilogram of concrete } [2].
\]

\[
D_{1} \text{ is the hydraulic conductivity (permeability) in Fick’s Law and } D_{2} = 0 \text{ is the coefficient for Soret mass flux which is usu-}
\]
ally neglected due to its small contribution. Hence the effective permeability can be given as \( D_1 = D_w + D_c \), in which \( D_w \) is the permeability of the uncracked material, \( D_w = f_1(h)10^{C_T(T - T_0)} D_0^w \), and \( D_c \) is the permeability due to the water flow in the cracks, formu-
lated by postulating a Poiseuille flow, \( D_c^j = \rho_c/(12\mu_c A_w) \sum_{i=1}^6 l_{NP_j}(\delta_{NP_j})^3 \), where \( f_1(h) \) is a function of the dynamic viscosity of the vapor-liquid mixture in cracks; \( \delta_{NP_j} \) denotes the facet normal crack openings on side \( T_i (i = 1, 2) \) in the FLE domain, \( j = 1, 2, 3 \); \( l_{NP_j} \) is the crack length on the \( P_iP_2P_3 \) surface (see in Fig. 2(c)).

\( D_4 \) is the thermal conductivity in Fourier’s Law and \( D_3 = 0 \) is the coefficient for Du-
four heat flux which is usually neglected due to its small contribution. As emphasized by Shen et al. \[16\], it is the cracks sub-orthogonal to thermal conduction, rather than the sub-parallel cracks, that have profound negative effect on concrete heat conduction performance. For this reason, the crack opening of 12 facets sub-orthogonal to FLE (Fig. 2(d)) are used to take into account the effect of fracture on the thermal conduction:

\[
D_4 = \frac{\lambda_t}{12} + \frac{\lambda_t}{\chi_{\text{NO}}} + \frac{\lambda_l}{\chi_{\text{NO}}} + \frac{\lambda_l}{\chi_{\text{NO}}}
\]

in which, \( \lambda_t^0 \) is the initial thermal conductivity of uncracked material; \( \delta_{\text{NO}}^i = \sum_{j=1}^6 \delta_{\text{NO}}^i/J_6 \) (\( i = 1, 2 \), \( j = 1, 2, 3 \)) is the average normal cracking opening of the 6 facets sub-orthogonal to FLE on each side \( T_i \); \( \lambda_c \) is the thermal conductivity of the vapor-liquid water mixture in the cracks.

\( w_c(p, T) \) and \( U_c(p, T) \) represent water mass and heat content per unit volume of cracked material and are calculated by the properties of the liquid-vapor water mixture in the cracks. These mixture properties are determined by the water state, because condensation and evaporation of free water might happen. If \( h > 1.1 \), water in the cracks is liquid. When \( h < 1 \), the water state is vapor. Otherwise, when \( 1 < h \leq 1.1 \), water is a mixture and the phase change is modeled by the smoothstep function. \( \chi_c = (\chi_l - \chi_v)\{ -2[10(h - 1)]^3 + 3[10(h - 1)]^2 \} + \chi_v \), in which \( \chi_c, \chi_l, \chi_v \) are parameters for the vapor-liquid mixture, vapor and liquid water, respectively. The same function \( \chi_c \) is used for \( \rho_c, C_c, \lambda_c, \) and \( \mu_c \) in which \( \rho_l, \rho_v, C_t, C_v, \lambda_t, \lambda_v, \mu_t, \mu_v \) can be found in \[17\].

3 Concrete thermal spalling mechanisms

This section analyzes the main mechanisms of concrete thermal spalling. The considered simulations setup (see in Fig. 3) is the one used in the experiments carried out by Lo Monte et al. \[12\]. In the numerical analyses a side length of 400 mm was used and, correspondingly, all other dimensions were scaled by 0.5. The heating load (Fig. 3) was applied on the central window (300×300 mm) and the displacements of the cold rim peripheral faces were set to zero. Since no information was available for the properties of the concrete used in the experiments, the parameters in Tab. 1 and Tab. 2 were used.

![Figure 3: Spalling thermal loads and experiment setup.](image-url)
era observations obtained by Zeiml et al. [4].

Table 2: Concrete mix-designs and model parameters used in the simulations

<table>
<thead>
<tr>
<th>Para.</th>
<th>Unit</th>
<th>Concrete Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mix-designs</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$c$</td>
<td>[kg/m³]</td>
<td>350 [11]</td>
</tr>
<tr>
<td>$w_{mix}/c$</td>
<td>[-]</td>
<td>0.5 [11]</td>
</tr>
<tr>
<td>$a/c$</td>
<td>[-]</td>
<td>5.23 [11]</td>
</tr>
<tr>
<td>$d_a$</td>
<td>[mm]</td>
<td>20 [11]</td>
</tr>
</tbody>
</table>

LDPM at room temperature

| $E_0$ | [MPa] | 43748 Identified |
| $\sigma_t$ | [MPa] | 4 Identified |
| $l_t$ | [mm] | 120 Identified |
| $\sigma_s$ | [MPa] | 10.8 Identified |
| $\sigma_{e0}$ | [MPa] | 150 Identified |
| $\mu_0$ | [-] | 0.2 Identified |
| $\sigma_{N0}$ | [MPa] | 600 Identified |
| $\kappa_{e0}$ | [-] | 2 [9] |
| $\kappa_{e1}$ | [-] | 2 [9] |
| $\kappa_{e2}$ | [-] | 1 [9] |
| $d_0$ | [mm] | 4 Assumed |

DTemPor3 model

| $w_0$ | [kg/m³] | 100 [2, 12] |
| $D_v^0$ | [m/s] | $8 \times 10^{-13}$ Identified |
| $\lambda_w^0$ | [W/(°C · m)] | 2 Identified |
| $C_T$ | [-] | 0.0045 Identified |

The same numerical analyses were carried out again by excluding the effect of pressure ($b = 0$ in Eq. [3]) or the effect of thermal expansion ($\alpha_T = 0$ in Eq. [1]). Fig. 4(c) shows the crack opening distribution after 30 minutes of heating if only thermal expansion is included. In this case the cracking distribution is similar to that of the complete simulation, but the spalling area is smaller and the generation of fragments is somewhat less pronounced. This indicates that thermal dilatation is a major contribution to generate damage inside the specimen and consequent spalling.

Fig. 4(d) shows the crack opening distribution after 30 minutes of heating if only the effect of pressure is included. In this case, a totally different cracking pattern occurs. A clear macro-crack is formed near the heating surface which cannot be found in Fig. 4(b) and much less micro-cracks are generated inside the specimen. The most important point is that no thermal spalling (fragment) is observed. In conclusion, it is clear that the effect of pressure is not enough to cause thermal spalling, but the formation of the macro-crack isolates a layer of concrete near the surface which is then more likely to buckle and to spall off if thermal stresses are present.

4 Conclusions

This study proposes a discrete 3D hygro-thermal model (DTemPor3) for concrete at high temperature coupled with the Lattice Discrete Particle Model (LDPM) for the simulation of thermal spalling. The two-way coupling simulations is equipped with the capability of taking into account the effect of cracks on heat transfer and mass transport as well as the cracking behavior caused by thermal expansion and pore pressure. This multi-physics framework is implemented into the MARS code [18].

By using the coupled the DTemPor3-LDPM framework, the numerical simulations reproduced successfully concrete thermal spalling. Thermal stresses play a dominant role in concrete thermal spalling. Thermal expansion supplies the major contribution to generate micro-cracks inside concrete. Pore pressure is not enough to form spalling, although pore pressure can form macro-cracks parallel to the heat surface which are then more likely to buckle and spall under the effect of thermal stresses.

REFERENCES


Figure 4: Crack opening contour during thermal spalling. (a) After 15 minutes of heating with all spalling factors included; (b) After 30 minutes of heating with all spalling factors included; (c) After 30 minutes of heating with only thermal stresses effect; (d) After 30 minutes of heating with only pressure effect.

ods in applied mechanics and engineering 195: 5707–5729.


