

PAPER • OPEN ACCESS

Thermodynamic modeling of Portland cement without mineral additives

To cite this article: Yu Abzaev *et al* 2019 *J. Phys.: Conf. Ser.* **1145** 012016

View the [article online](#) for updates and enhancements.

You may also like

- [Numerical investigation of the external sulfate attack induced expansion response of cement paste by using crystallization pressure](#)
Guang-Ji Yin, Xiao-Bao Zuo, Xiang-Hua Sun *et al.*
- [Review on recent advances in securing the long-term durability of calcium aluminate cement \(CAC\)-based systems](#)
Hayeon Kim, H M Son and H K Lee
- [Preparation and characterization of Portland cement clinker from sulfuric acid leaching residue of coal fly ash](#)
Aichun Zhao, Yujin Liu, Ting-an Zhang *et al.*



ECS
The
Electrochemical
Society
Advancing solid state &
electrochemical science & technology

DISCOVER
how sustainability
intersects with
electrochemistry & solid
state science research

Thermodynamic modeling of Portland cement without mineral additives

Yu Abzaev, A Gnyrya, S Korobkov¹, K Gauss, A Boyarintsev, S Tomrachev

Construction Engineering Technology Department, *Tomsk State University of Architecture and Building*, 2 Solyanaya Square, Tomsk, 634003, Russian Federation

¹E-mail: korobkov_1973@mail.ru

Abstract. The paper deals with thermodynamic modeling of Portland cement hydration as a complex system, which describes the clinker dissolution, diffusion, and surface phenomena that occur on phase nuclei at different water/cement ratio and depend on the curing time and temperature of the whole process. Using Gibbs Energy Minimization Software (GEMS) and the hydration model proposed by Parrot and Killoh, thermodynamic modeling allows a long-term detection of the amount of both original clinker and nucleating phases such as cement paste, ettringite, Portlandite, and others. The paper presents results of GEMS modeling the phase composition during Portland cement hydration in terms of the Parrot and Killoh model and using the Rietveld refinement technique. Alite, belite, ferrite, and aluminate phases predominate in the cement paste. In order to get the Gibbs free energy of Portland cement in the vicinity of the cement system equilibrium, GEMS modeling considers a balance between the dissolution rate of clinker phases and the deposition of solid solutions of individual phases using thermodynamic parameters at different stages of cement hardening. At the initial stages of hydration, the aqueous solution is oversaturated relative to the amount of elements which determine the Portlandite and ettringite compositions. During the hydration process, the formation of stable complex hydrated silicates occurs, and pH value decreases. It is found that the main components of hardening Portland cement are calcium–silicate–hydrate (C–S–H) and Portlandite which are used herein as reference phases for the identification of their content in Portland cement. Major phases of Portland cement after 5-month curing are studied using the Rietveld method as a tool of the quantitative phase analysis. As a result, the following phase composition is identified: 47.72% tobermorite amorphous phase, 37.40% ettringite, 5.12% portlandite, 0.30% alite and 7.96% belite. The obtained experimental data are in good agreement with theoretical calculations. *Ab initio* assessments of the binding energy prove the lattice stability in detected major phases.

1. Introduction

In different concrete types hydrated cement paste is the main binding material. The structure modification of Portland cement at different stages of curing is a complicated, top-down, multi-stage process which includes stages of active chemical reactions, diffusion processes and curing [1–2]. The main components of Portland cement are calcium silicates C_3S and C_2S , aluminate C_3A and ferrite C_4AF . Such components as calcite, calcium oxide, magnesium oxide, sodium and potassium sulphates are also present. During the hydration process, these components react with water and form various products, namely: calcium–silicate–hydrate (C–S–H), ettringite, Portlandite, calcium monosulfoaluminate and calcium monocarbonate. Thermodynamic modeling utilizes GEMS software



[3-5] to predict the quantitative content of Portland cement hydration products with a glance to the curing time and temperature observed during chemical reactions and diffusion and hardening processes. Consequently, hydration products can be used as reference phases for the Rietveld quantitative identification of their content in Portland cement. Within one process, it is possible to vary such parameters as the phase composition, water/cement ratio, temperature, hydration time, *etc.* This provides a long-term prediction of the hydrated system composition at different temperatures. Apparently, the modeling results represent a quantitative basis for the investigation of structural and mechanical properties of individual products and Portland cement as a whole system at various curing stages and temperatures. In terms of Gibbs Energy Minimization Software (GEMS) modeling, lattices of hydration products are assumed to be stable. This assumption requires additional confirmation. If the structural information (parameters, orientation, space group, *etc.*) about the major phase lattices is known, the lattice stability in these phases relative to the delamination into pure components can be determined from *ab initio* calculations.

It is rather relevant to study the quantitative phase content of Portland cement during its curing. Studies are performed *via* GEMS modeling [3-6] and using the Rietveld refinement technique for Portland cement having a composition matching the type CEM I 42,5B Portland cement manufactured in OOO ‘Topkinskii cement’ (Topki, Kemerovo region, Russia). In the works of Lothenbach, Matschei, Winnefeld, Möschner, Glasser, [7-11] and others, GEMS software was adapted to hydration of cement systems in terms of the Parrot and Killoh model [12].

A thermodynamic approach implemented by GEMS modeling, provides the quantification of the weight content of hydration products and pH value description over a long period of time. A description of modeling given in [5-11] is in a good agreement with the experimental results. The X-ray phase analysis is carried out by DRON-4-07 diffractometer. Measurements are conducted using copper radiation (K_{α}) and Bragg-Brentano X-ray optical scheme. Specifications for the DRON-4-07 include 0.02° scanning step; $14-71^{\circ}$ range for angles to be scanned; 30 kV voltage; and 25 mA current. The quantitative phase analysis (QPA) of Portland cement is based on the Rietveld method.

The aim of this work is to perform thermodynamic GEMS modeling of the quantitative phase composition of Portland cement during the hydration process at various temperatures. The composition of Portland cement is close to that of binding materials in heavy concretes without mineral additives. In this experiment, we investigate Portland cement manufactured in OOO ‘Topkinskii cement’ [13-15].

2. Material and model approximation

The type CEM I 42.5B Portland cement [13-15] was used in this experiment to determine its weight content. This type of Portland cement is used in manufacturing heavy concretes with high performance properties. In accordance with the quality certificate of OOO ‘Topkinskii cement’ (Topki, Kemerovo region, Russia), the chemical composition and the weight content of Portland cement were ascertained and summarized in table 1.

Data presented in table 1 are used to provide the Bogue calculation of the mineralogical composition in Portland cement clinker [16]. In GEMS modeling, thermodynamic calculations of the mass balance in Portland cement clinker are normalized to 100 grams of weight. Therefore, 100 g of Portland cement contain approximately 61.06 and 13.62 g of calcium silicates, respectively for C_3S and C_2S , 12.79 g of ferrite and 6.50 g of aluminat. Also, there are 41.0 g of water and 0.34 g of oxygen which are used to simulate the hydration process. Data presented in this table are the input parameters for GEMS modeling the hardening process of Portland cement [3-6].

Table 1. Composition of Portland cement CEM I 42.5B.

Phase	Content, wt. %	Mineral	Weight, g
SiO ₂	20.49	C ₃ S	61.06
Al ₂ O ₃	5.06	C ₂ S	13.62
Fe ₂ O ₃	4.14	C ₄ AF	12.79
CaO	62.83	C ₃ A	6.50
MgO	1.75	Aqueous solution	41
Na ₂ O	0.34	O ₂	0.34
K ₂ O	0.65	MgO	1.78
SO ₃	3.10	K ₂ O	0.66
–	–	Na ₂ O	0.34
–	–	SO ₃	3.15

In order to get the Gibbs free energy of Portland cement in the vicinity of the cement system equilibrium, GEMS modeling considers a balance between the dissolution rate of clinker phases and the deposition of solid solutions of individual phases using thermodynamic parameters at different stages of cement hardening. Experimental equations for the Parrot and Killoh model [12] refined by Lothenbach [11] are as follows.

$$R_{i,T} = \frac{K_1}{N_1} \cdot (1 - \alpha_t) \cdot (-\ln(1 - \alpha_t))^{1-N_1} \cdot \left(\frac{rh - 0.55}{0.45}\right)^4 \cdot \frac{S}{385} \exp\left(-\frac{E_a}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right) \quad (1)$$

$$R_{i,T} = \frac{K_1 \cdot (1 - \alpha_t)^{2/3}}{1 - (1 - \alpha_t)^{1/3}} \cdot \left(\frac{rh - 0.55}{0.45}\right)^4 \exp\left(-\frac{E_a}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right) \quad (2)$$

$$R_{i,T} = K_3 \cdot (1 - \alpha_t)^{N_3} \cdot \left(\frac{rh - 0.55}{0.45}\right)^4 \exp\left(-\frac{E_a}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right), \quad (3)$$

where E_a is the activation energy of dissolution; rh is the degree of the system closing (when $rh = 1$, the system is closed); T , T_0 are respectively current and room temperatures; S is the surface area of phase nucleus; α_t is the degree of hydration which can be obtained from the following recurrent equation:

$$\alpha_t = \alpha_{t-1} + \Delta t \cdot R_{t-1} \left[1 + 3.333 \cdot (H\mu - \alpha_t)\right]^4, \quad (4)$$

where μ is the water/cement ratio. The hydration process develops when $(H\mu - \alpha_t) < 0$. Another parameters of the Parrot Killoh and Lothenbach model are given in table 2.

Equations (1)–(3) describe the following stages: 1) nucleation and development of phases (equation (1)); 2) diffusion processes (equation (2)). Phenomenological dependences of reaction rates and hydration parameters are obtained for each clinker phase [3-4, 6, 12]; 3) hydration degree (equation (3)). The water/cement ratio, humidity and specific surface of phase nuclei are also considered.

When contacting with water, alkali-metal sulphates dissolve and release K, Na and S into a liquid phase. At a slow hydration of clinker components, the formation of such elements as Ca, Si, Al and Fe occurs, and hydroxides also emerge. The formation of these elements in this solution occurs after the dissolution of the respective clinker structure.

Table 2. Parameters of Parrot, Killoh and Lothenbach.

Parameter	Alite	Belite	Aluminate	Ferrite
K ₁	1.5	0.5	1.0	0.37
N ₁	0.7	1.0	0.85	0.7
K ₂	0.05	0.006	0.04	0.015
K ₃	1.1	0.2	1.0	0.4
N ₃	3.3	5.0	3.2	3.7
H	1.33	1.33	1.33	1.33

Alkalies emerging during the dissolution of alkali-metal sulphates distribute between this solution and C–S–H solid solution. Ca and Si elements react with C–S–H solid solution which is the main product of the interaction between the solid and liquid phases. The concentration of alkalies is rather low as compared to that of Ca and Si elements. Al and Fe elements react with hydroxides. The dissolution of clinker phases is determined by the amount of Ca, Si, Al and Fe elements and hydroxides. In turn, the dissolution of clinker phases determines the rate of deposition of major hydrated phases, namely C–S–H and calcium–aluminosilicate–hydrate (C–A–S).

3. Results and discussion

GEMS modelling includes hydration of Portland cement during the time period ranging from 0 to 1000 days at a room temperature, which is illustrated in figure 1*a, b*. The temperature dependence is suggested between the weight content of individual phases at a final stage of the hydration process within a 4–95 °C temperature range, during which the aqueous solution continues to be liquid. We study the temperature effect on pH value at 5–95 °C as depicted in figure 1*c, d*.

As a results of GEMS modeling, the following phases are found at a room temperature which are present in a thermodynamic equilibrium: free moisture; C₃(AF)S_{0.84}H; CSHQ; ettringite; alite; belite; ferrite; aluminate; portlandite; goethite; arcanite; OH-hydrotalcite. We determine the amount of free moisture, gas, pH value and solid formations appeared during the hydration of the above-listed phases. The Parrot and Killoh model is used to obtain the dependence between the amount of alite, belite, ferrite and aluminate phases and the time of hydration [12]. It is supposed that free moisture occupies the voids volume of Portland cement.

The elements presenting in the aqueous solution at different hydration time are summarized in table 3. According to this table, during the first 1.6–2 h, ions of Ca⁺², K⁺, Mg⁺², Na⁺ and OH⁻ predominate. A high concentration of K⁺, Mg⁺² and Na⁺ ions is conditioned by the rapid dissolution of alkali and sulphate phases. The effective ionic strength of the solution decreases. The amount of K⁺, Na⁺ and OH⁻ ions and the ionic strength substantially increase with time. The main body of natrium and potassium enters eventually the solution, except for those elements which adsorb on C–S–H grains. The amount of Ca in the solution continues to be stable for 6–7 h and then rapidly decreases. Concentration of OH⁻ hydroxide gradually grows, weakly changes within a 1.6–6.5 h period, and then rapidly increases even regardless of the growth in portlandite concentration. This is depicted in figure 1*a, b*. Experiments show that alkali-metal sulphates completely dissolve in the liquid solution, whereas sulphuric anhydride SO₃ dissolves partially until the equilibrium state is achieved in the solution. As can be seen from figure 1, the amount of free moisture considerably lowers with time. As a result of the particle dissolution of the clinker minerals, new formations appear, namely hydrates of (CaO)_x*(SiO)_y*(H₂O)_z*Ca(OH)₂.

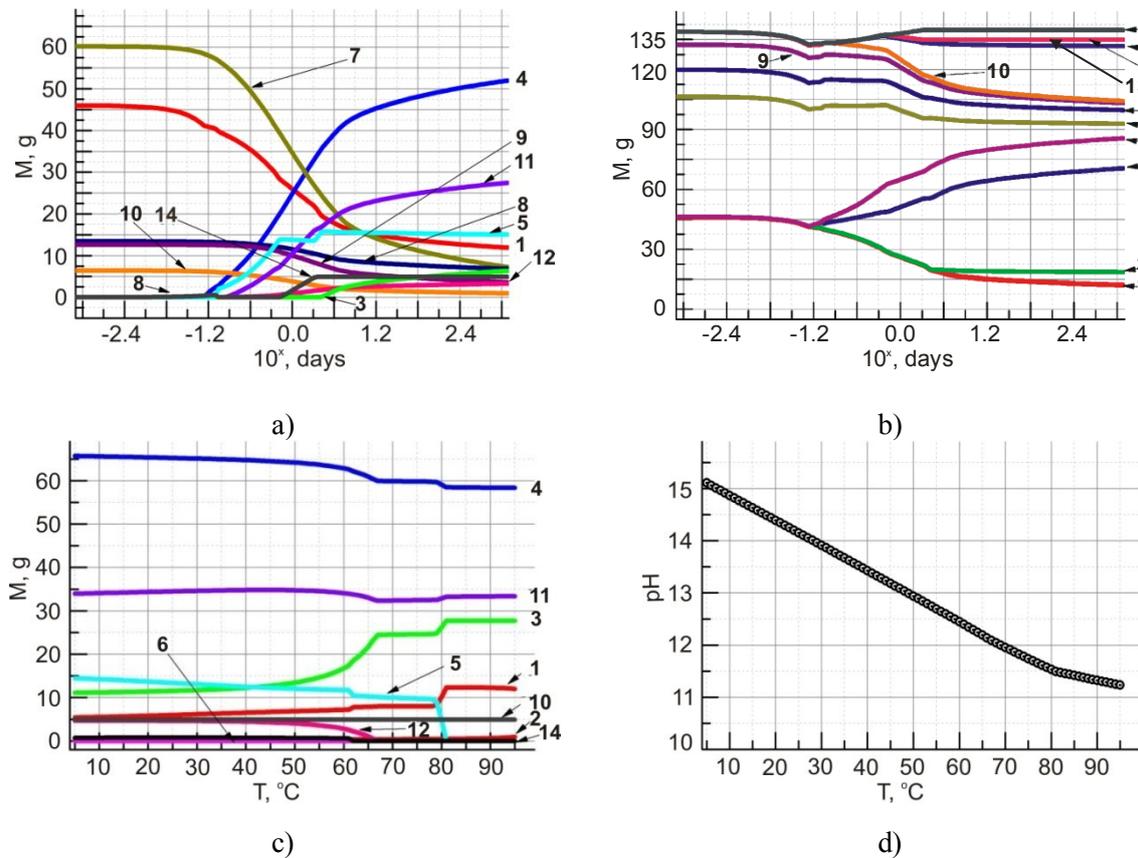


Figure 1. Time (a) and cumulative (b) dependences between weights of hydration products of Portland cement individual phases; temperature dependence of hydration products of Portland cement individual phases within 0–95 °C (c); temperature dependence of pH value in aqueous solution (d): 1 – free moisture; 2 – gas; 3 – $C_3(AF)S_{0.84}H$; 4 – CSHQ; 5 – ettringite-Al; 6 – ettringite-Fe; 7 – alite; 8 – belite; 9 – ferrite; 10 – aluminate; 11 – portlandite; 12 – goethite; 13 – arcanite; 14 – OH-hydrotalcite.

The product of the interaction is a new C–S–H phase. The liquid phase also comprises ions of aluminum and iron (in a low concentration) which enable the formation of hydrated calcium aluminates and hydrated calcium ferrites. During the hydration process, sulphate deposits in the form of ettringite. At the initial stages of the hydration process, the aqueous solution is oversaturated as compared to the amount of elements in the composition of portlandite and ettringite. C_3S and C_2S phases are metastable at the initial stages, whereas later they transfer to stable complex hydrated silicates of $(CaO)*(SiO)*(H_2O)$. Owing to weak crystallization of hydration products and large amount of mixing water, they are called cement gel. Hydrated silicates is the main binding material in moistened cement. The quantitative phase composition is in good agreement with results obtained in works of [9, 10], given that monocarbonates and monosulfates are absent.

The hydrated system modeling produces the following results. During 36–40 min, the reduction is observed in the content of free moisture (by 4.2 g), alite (by ~2 g), belite (by ~0.14 g), aluminate (~0.2 g), and ferrite (~0.03 g) (figure 1b). The initial formation of C–S–H is detected. The formation of anhydrite and portlandite starts after ~1.0 h and 1.4 h, respectively. The stable formation of OH-hydrotalcite in the amount over 0.33 g is observed after 8.6 h curing. $C_3(AF)S_{0.84}H$ phase forms after 32.7 h curing and then monotonously increases up to 6.32 g up to the end of the experiment. The total weigh of the system is 153.87 g by the end of the hydration process.

Table 3. Elements in aqueous solution at different hydration time.

Hours	Millimoles								Ionic strength
	Ca ⁺²	K ⁺	Mg ⁺²	Na ⁺	O ₂	OH ⁻	SiO ₂	SiO ₃ ⁻²	
0.02	1.09	238.93	280.86	205.44	0.79	0.14	0.11	0	1.71
0.05	2.759	229.27	276.92	206.00	0.79	0.15	0.11	0	1.69
1.0	4.69	293.22	0	242.66	1.03	24.93	0	0.21	1.69
1.6	5.36	311.88	0	253.75	1.03	111.48	0	0.05	0.76
2.0	5.27	324.04	0	263.97	1.02	112.54	0	0.05	0.78
4.0	5.08	351.12	0	287.32	0.998	114.70	0	0.00	0.86
6.5	3.97	381.3	0	317.67	0.98	129.71	0	0.08	0.93
8.6	0.39	439.01	0	339.25	0.98	415.73	0	0.08	0.91
16.8	0.35	501.42	0	389.12	0.95	434.78	0	0	1.05
29.7	0.09	0617.43	0	447.85	0.92	835.30	0	0.38	1.05
93.3	0.050	775.71	0	545.85	0.86	1097.83	0	0.76	1.38
690	0.04	877.74	0	616.37	0.81	1173.67	0	0.96	1.59
1480	0.04	910.31	0	639.17	0.80	1193.22	0	1.03	1.65
14584	0.03	993.74	0	698.40	0.76	1232.66	0	1.20	1.82

The deposition of C₃(AF)S_{0.84}H phase lasts for 4.89 h. Its content monotonously grows up to 6.33 g. The total content of alite, belite, aluminate and ferrite clinker phases decreases 4 times, *i.e.* from 92.55 to 18.63 g. Hydration products include C–S–H, portlandite, ettringite, C₃(AF)S_{0.84}H, OH-hydroxalcite, and goethite. Their weight is respectively 51.97; 27.47; 15.02; 6.33; 4.9 and 3.27 g. The amount of free moisture which occupies the voids volume of Portland cement equals 11.9 g. It is important to note the increase of pH value during the hydration process, which achieves 12.94 as shown in figure 1. Gas release in the system is insignificant, only 0.3044 g.

The weight content of hydration products after 28 days (672 h) is also of particular interest. Thus, the weight contents of C–S–H, portlandite, ettringite, C₃(AF)S_{0.84}H, OH-hydroxalcite and goethite are respectively 46.51; 23.9; 15.39; 4.17; 4.90 and 2.74 g. The amount of alite, belite, aluminate, ferrite phases and water is 12.91; 8.01; 5.06; 1.5 and 14.39 g, respectively. These findings show that the main cement components are C–S–H, portlandite and ettringite. It is worth noting that the volume fractions of the main hydration products continue to grow until 1000 days of curing (figure 1). Thermodynamic modeling combined with hydration rates calculated in GEMS [3-4, 6], predicts the anhydrite degradation approximately after 6 h of curing and the decrease in sulphate concentration in aqueous solution. This is because ettringite deposits until the sulphate content is present in the solution. After the initial stage, when pH value of the solution is maintained, the value of pH increases. This results in the reduction in Ca concentration due to the total ion effect, whereas the estimated concentrations of Al, Si and Fe grow with the decrease in moisture.

Figure 1c contains the temperature dependence of Portland cement hydration within a 5–95 °C temperature range. It is important to note that at these temperatures, pH value considerably lowers with the temperature growth (figure 1d). At 5 °C, the solid fraction comprises 65.69 g of C–S–H, 39.95 g of portlandite, 14.47 g of ettringite, 11.09 g of C₃(AF)S_{0.84}H, 4.90 g of OH-hydroxalcite and 4.67 g of goethite. Aqueous solution amounts to 5.42 g by the end of the hydration process. With the temperature increase, the phase content in the solid fraction reduces. Thus, at 66 °C, C–S–H constitutes 60.40 g, portlandite – 32.66 g, ettringite – 10.47 g and no goethite. The amount of OH-hydroxalcite does not change (4.90 g), while the content of C₃(AF)S_{0.84}H reaches 23.17 g at 66 °C and 27.68 g at 95 °C. A further temperature increase enables the growth in the portlandite content up to 33.36 g, but C–S–H content reduces down to 58.33 g. Starting from 66 °C, the gas amount increases up to 0.91 g. The amount of the voids volume in Portland cement increases almost twice.

Table 4 summarizes the QPA results on the phase composition in Portland cement after 5-month curing at room temperature. The phase composition includes clinker phases, hydration products, and

amorphous phase which is used to measure the X-ray pattern background. Tobermorite and ettringite lattices include H₂O molecules. A full structural information is obtained for all the phase lattices, including the amorphous phase. The QPA analysis shows that such hydration products as tobermorite, ettringite, tobermorite amorphous phase and portlandite predominate in Portland cement. There are also clinker minerals of alite and belite. The QPA results match the results of GEMS modeling.

Table 4. QPA results on phase composition of Portland cement after 5-month curing.

Phases	Tobermorite	Amorphous	Ettringite	Alite	Belite	Portlandite
Phase composition, %	47.72	-	37.40	0.30	7.96	5.12
Lattice energy, eV	-61216.54	-65463.99	-72504.21	-31868.08	-934.85	-1911.72
Binding energy, eV	-2335.69	-2281.27	-934.85	-934.86	-391.19	-65.02

According to Table 4, *ab initio* calculations of the lattice energy and stability in major phases at 0 K [17] show that the lattice and binding energies, including the amorphous phase, are negative. The binding energy for the lattices under study, except for Portlandite, achieves several hundred electronvolts. The lattices of clinker phases and hydration products are observed to be in a high-stable state relative to the delamination into pure components.

4. Conclusion

This paper has clearly shown that the curing process of the cement paste was rather complex. The time and temperature of curing had a significant effect on the quantitative content of hydrated silicates. The QPA results showed that the main hydration products of Portland cement were tobermorite amorphous phase (both in crystalline and amorphous states), portlandite and ettringite. Their weight content continued to increase until 1000 days of curing. However, the intensity of their accumulation lowered after 28 days. The amount of C-S-H was the highest (over 60%) and reduced with the temperature increase. The QPA results also showed the presence of alite and belite, but the content of the former is insignificant. The major phase lattice was dynamically stable at 0 K that was confirmed by *ab initio* calculations. GEMS modeling of the hydration process of cements having various compositions, element content in aqueous solution, pH value, water/cement ratio, initial phase compositions can be used to intensify the performance characteristics of Portland cement and reduce the curing time of the cement paste nearby the thermodynamic equilibrium and within a wide temperature range.

Acknowledgments

Authors wish to acknowledge the financial support from the Russian Foundation for Basic Research (Grant No 18-08-01025).

References

- [1] Matschei T 2007 *Thermodynamics of cement hydration*, DSc thesis, University of Aberdeen
- [2] Liu Z, Sha A, Hu L, Lu Y, Jiao W, Tong Z and Gao J 2017 Kinetic and thermodynamic modeling of Portland cement hydration at low temperatures *Chem. Pap.* **71** 741
- [3] Kulik D A, Wagner T, Dmytrieva S V, Kosakowski G, Hingerl F F, Chudnenko K V and Berner U 2013 GEM-Selektor geochemical modeling package: revised algorithm and GEMS3K numerical kernel for coupled simulation codes *Computat. Geosci.* **17** 1
- [4] Wagner T, Kulik D A, Hingerl F F and Dmytrieva S V 2012 GEM-Selektor geochemical modeling package: TSolMod library and data interface for multicomponent phase models

Can. Mineral. **50** 1173

- [5] Lothenbach B, Le Saout G, Ben Haha M, Figi R and Wieland E 2012 Hydration of a low-alkali CEM III/B–SiO₂ cement (LAC) *Cem. Concr. Res.* **42** 410
- [6] *GEM Software (GEMS) Open Database*, available at: <http://gems.web.psi.ch/termsfuse.html>
- [7] Ben Haha M, Le Saout G, Winnefeld F and Lothenbach B 2011 Influence of activator type on hydration kinetics, hydrate assemblage and microstructural development of alkali activated blast-furnace slags *Cem. Concr. Res.* **41** 301
- [8] Pelletier-Chaignat L, Winnefeld F, Lothenbach B and Müller C J 2012 Beneficial use of limestone filler with calcium sulfoaluminate cement *Constr. Build. Mater.* **26** 619
- [9] Winnefeld F and Lothenbach B 2010 Hydration of calcium sulfoaluminate cements – experimental findings and thermodynamic modelling *Cem. Concr. Res.* **40** 1239
- [10] Lothenbach B, Le Saout G, Gallucci E and Scrivener K 2008 Influence of limestone on the hydration of Portland cements *Cem. Concr. Res.* **38** 848
- [11] Lothenbach B, Matschei T, Möschner G and Glasser F P 2008 Thermodynamic modelling of the effect of temperature on the hydration and porosity of Portland cement *Cem. Concr. Res.* **38** 1
- [12] Parrot L J and Killoh D C 1984 Prediction of cement hydration *Proc. Br. Ceram. Soc.* **35** 41
- [13] *Standard cements* [in Russian – Obshchestroitel'nye tsementy], available at: www.sibcem.ru/index.php/production/cement/obshchestroitelnye-tsementy
- [14] Gnyrya A, Abzaev Y, Korobkov S, Mokshin D, Gauss K and Boyarintsev A 2017 High-temperature structure formation in cement depending on curing time *AIP Conf. Proc.* **1899** 040005
- [15] Gnyrya A I, Abzaev Yu A, Korobkov S V, Boyarintsev A A, Mokshin D I and Gauss K S 2017 Influence of time and increased temperature on structural creation of cement stone *News of Higher Educational Institutions. Construction* [Izvestiya Vysshikh Uchebnykh Zavedenii: Stroitel'stvo – in Russian] **8** 34
- [16] Taylor H F W 1989 Modification of the Bogue calculation *Adv. Cem. Res.* **2** 73
- [17] Abzaev Yu A, Syzrantsev V V and Bardakhanov S P 2017 Simulation of the structural state of amorphous phases in nanosclae SiO₂ synthesized via different methods *Physics of the Solid State* [Fizika tverdogo tela – in Russian] **59** 1874