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**MATHEMATICAL MODELING OF HEAT AND MASS TRANSFER
IN SINTER LAYER**

The article is devoted to the mathematical simulation of interconnected physical processes on sintering machine during agglomeration of iron ore pellets. The mathematical model uses system of partial differential equations and takes into account velocity of a horizontal movement of the layer and a vertical velocity of the air movement through the layer as well as phase transition and chemical reactions of pellet components. The purpose of the simulation is getting the time dependency of sinter and gas temperature and concentration of their components, distributed by length and height of the layer, to find rational parameters of the process further. A numerical experiment shows that the temperature front, which is lower in the layer cross-section, has a larger gradient in comparison with the upper front, where the finished agglomerate is cooled, because the water takes much energy to evaporate. The obtained results are consistent with the literature data.

Keywords: mathematical model, ore sintering, thermodynamics, mass transfer, system of partial differential equations, explicit scheme.

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**МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ТЕПЛОМАСОПЕРЕНОСУ
В АГЛОМЕРАЦІЙНОМУ ШАРІ**

Стаття присвячена математичному моделюванню взаємопов'язаних фізичних процесів на агломераційній машині при спіканні гранул залізної руди. Агломераційні машини достатньо розповсюджені використовуються на металургійних комбінатах, що дає підстави для економічного ефекту від оптимізації процесу. Агломераційний шар розглядається як суцільне середовище, яке складається з різних субстанцій, концентрація яких змінюється у ході фізико-хімічних реакцій. Геометрія шару дозволяє використовувати Декартову систему координат. Математична модель використовує систему диференціальних рівнянь у частинних похідних і враховує швидкість горизонтального руху шару та вертикальну швидкість руху повітря через шар, а також фазовий перехід і хімічні реакції компонентів гранул. Мета моделювання полягає в одержанні часової залежності температури агломерату, газу та концентрацію їх компонентів, розподілених за довжиною і висотою шару, для пошуку раціональних параметрів даного процесу. Рівняння розв'язуються чисельно, розбиваючи часову вісь кроками, на кожному з яких стан системи визначається через попередній. Чисельний експеримент показав, що температурний фронт, який розташований нижче в поперечному перерізі, має більший градієнт у порівнянні з верхнім фронтом, де готовий агломерат охолоджується, оскільки вода потребує значної енергії для випаровування, що суттєво впливає на перебіг процесу. Основним джерелом теплової енергії є кокс, який міститься в шихті. Під час його горіння високотемпературний фронт рухається вниз і по довжині шару, підпалюючи нові частинки коксу. Після спікання агломерат поступово охолоджується до необхідної температури. Отримані результати відповідають літературним даним, але для більш кращого наближення у подальшому треба було б окремо враховувати втрати тепла від стінок агломераційної машини, додаючи відмінність температури і концентрації речовин по ширині шару шихти, таким чином модель стане тривимірною у просторі.

Ключові слова: математична модель, агломераційна машина, спікання руди, термодинаміка, масоперенос, диференціальні рівняння у частинних похідних, явна схема чисельного розв'язку.

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**МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ТЕПЛОМАСОПЕРЕНОСА
В АГЛОМЕРАЦИОННОМ СЛОЕ**

Статья посвящена математическому моделированию взаимосвязанных физических процессов на агломерационной машине при спекании гранул железной руды. Математическая модель использует систему дифференциальных уравнений в частных производных и учитывает скорость горизонтального

движения слоя и вертикальную скорость движения воздуха через слой, а также фазовый переход и химические реакции компонентов гранул. Цель моделирования состоит в получении временной зависимости температуры агломерата, газа и концентрацию их компонентов, распределенных по длине и высоте слоя, для поиска рациональных параметров данного процесса. Численный эксперимент показал, что температурный фронт, который расположен ниже в поперечном сечении, имеет больший градиент по сравнению с верхним фронтом, где готовый агломерат охлаждается, поскольку вода требует значительной энергии для испарения. Полученные результаты соответствуют литературным данным.

Ключевые слова: математическая модель, агломерационная машина, спекание руды, термодинамика, массоперенос, дифференциальные уравнения в частных производных, явная схема численного решения.

Problem definition

Nowadays more than a half of steel production uses the sinter as resource for loading of blast furnace. Lengthy agglomeration machine, which is used for sinter production, firstly heats the layer of pellets using gas-burners and then cools ready agglomerate. From the practical point of view the scientists is interested in mathematical modeling of this process to determine the state of the sinter inside the layer in a various points of time and to search for the rational parameters of the process saving resources eventually.

Related publications

Authors of work [1] presented: a mathematical model of agglomeration process that described by system of a differential equations including coke's average diameter decreasing and sinter temperature changing; drawings with visualization of calculation results; operation parameters of the agglomachine, which can be used in testing of a mathematical model. Some of multipliers in equations do not depend on temperature and the values of the terms in the equations for the heat is not described well, so model can be improved.

In paper [2] the authors performed a detailed analysis of the computational results based on the mathematical model developed in [1] with plots of the temperature, the amount of melt, concentration of FeO and gases (O₂ and CO₂) along the length and height of the sinter layer. A number of recommendations are given to increase the specific productivity of sinter plants.

In work [3], a detailed review of the mathematical models of the sintering is made. The authors point out the need to improve considered models taking into account such important parameters as the layer height, the moisture of the sinter, its granulometric composition, carbon concentration, etc., which will allow technologists to consider a wider range of situations encountered in practice.

The authors of [4] offer a detailed description of the sintering process on the agglomeration machine, starting with the ignition stage, paying attention to temperature, moisture concentration in the layer, rarefaction in vacuum chambers and the sinter cooling.

At the conference ITMM-2017 [5] there was reported on existing mathematical models of agglomeration and was noted the need to take into account the speed of air movement with oxygen and water vapor through the sinter layer in the mathematical model.

Author of the works [6, 7] considers convection and diffusion of chemical substances, momentum, and energy in three dimensions taking into account phase transitions in partial differential equations. They are solved for steady state. Also it is needed unsteady solution to fully understand of the sinter state changes depending on time.

Agglomeration process includes air motion through sinter layer with speed, which depends on the sinter permeability. In work [8] author analyzes this permeability in case of sinter components melting considering basicity. Author of the work [9] proposes one-dimensional unsteady mathematical model of mass and heat transport in fixed sinter layer considering evaporation and condensation of moisture.

Article [10] devoted to mathematical description of heat transfer coefficient taking into account set of chemical reactions of the sintering process.

Authors of the works [11, 12] predict temperature inside sinter layer depending on time taking into account coke combustion rate. Also details of coke combustion are presented in [13] considering homogeneous, heterogeneous reactions and the heat exchange between solid and gas phases.

In thesis [14] among other things the author notes importance of sufficient temperature level for sintering process: low temperature is not enough; very high temperature causes excessive melting of layer and decreasing of its permeability.

Author of works [15, 16] models heat process inside sinter layer using finite volume method taking into account carbonates and hydrates dissociation. It is presented the plot of air speed and total amount of heat depending on layer height.

In works [17, 18] authors describes details of agglomeration process including water phase transition, concentration change of air and sinter components, coke combustion, sinter melting and crystallization. Authors presented figures which show result of experiments.

Articles [19, 20] devoted to peculiarities of gas circulation involved in sintering process. It is presented and compared temperature distributions for two technologies — FGRS and CS.

Goal of research

It is necessary to calculate the temperature distribution along the height and length of the layer, taking into account the change in the concentrations of the gas and the layer during the physicochemical reactions of carbon burning, iron oxidation, decomposition of calcium carbonate, evaporation and condensation of water, melting and crystallization of the sinter.

Presentation of the research material

It is assumed that the layer retains volume, and the sinter is a continuous medium. The geometry of a sinter layer, which has length about 30 meters and height – 0.5 meters, allows us to use Cartesian system of coordinates. The mathematical model includes a system of differential equations and additionally takes into account the influence of chemical reactions on the temperature distribution in the layer. Below the equations are supplemented by the initial and boundary conditions.

The change in the oxygen concentration in the air, which vertically passes through the layer:

$$\frac{\partial M_{O_2}}{\partial t} + v_z \frac{\partial M_{O_2}}{\partial z} = -m_{rO_2}, \tag{1}$$

The change in the FeO concentration in the layer:

$$\frac{\partial M_{FeO}}{\partial t} = -m_{rFeO}, \tag{2}$$

The change in the carbon concentration in the layer:

$$\frac{\partial M_C}{\partial t} = -m_{rC}, \tag{3}$$

The change in the water`s vapor concentration in the air:

$$\frac{\partial M_{H_2Og}}{\partial t} + v_z \frac{\partial M_{H_2Og}}{\partial z} = m_{riH_2O} - m_{rkH_2O}, \tag{4}$$

The change in the water concentration in the layer:

$$\frac{\partial M_{H_2O}}{\partial t} = m_{rkH_2O} - m_{riH_2O}, \tag{5}$$

The change in the CaCO₃ concentration in the layer:

$$\frac{\partial M_{CaCO_3}}{\partial t} = -m_{rCaCO_3}, \tag{6}$$

The change in the air temperature:

$$\frac{\partial T_{gas}}{\partial t} + v_z \frac{\partial T_{gas}}{\partial z} = -Q_{tob}, \tag{7}$$

The change in the sinter temperature:

$$\frac{\partial T_s}{\partial t} - a\Delta T_s = Q_{tob} + Q_{gC} + Q_{gFeO} - Q_{dCaCO_3} - Q_{iH_2O} + Q_{kH_2O} - Q_{pl} + Q_{kr}, \tag{8}$$

For the equations the boundary condition on the layer bottom, which is exit for the air, is the free passing of flux, so:

$$T_{\text{gas}}\Big|_{\text{bottom}} = 0, M_{\text{O}_2}\Big|_{\text{bottom}} = 0, M_{\text{H}_2\text{Og}}\Big|_{\text{bottom}} = 0$$

For the layer top the boundary condition depends on the state of the entering air, which is heated by gas-burners only at the beginning of machine and is cooled at the defined part of remaining top surface of the layer:

$$T_{\text{gas}}\Big|_{\text{top}} = \begin{cases} 1200, & \text{if } d \leq 2m \\ 50, & \text{if } d > 2m \end{cases}, M_{\text{O}_2}\Big|_{\text{top}} = 0.3$$

$$M_{\text{H}_2\text{Og}}\Big|_{\text{top}} = 0.01$$

In the above equations: a — coefficient of thermal conductivity, W/m/K; m_{rC} — amount of reacted carbon, kg/m³/s; m_{rFeO} — amount of reacted FeO, kg/m³/s; m_{rO_2} — amount of reacted oxygen, kg/m³/s; $m_{\text{rH}_2\text{O}}$ and $m_{\text{rkH}_2\text{O}}$ — amount of evaporated and condensed water respectively, kg/m³/s; m_{rCaCO_3} — amount of dissolved carbonate, kg/m³/s; Q_{tob} — change in the temperature of the sinter due to heat transfer from the air to the sinter, K/s; Q_{gC} and Q_{gFeO} — change in the temperature of the sinter from combustion of carbon and FeO respectively, K/s; Q_{dCaCO_3} — change in the sinter temperature from CaCO₃ dissolution, K/s; $Q_{\text{rH}_2\text{O}}$ and $Q_{\text{cH}_2\text{O}}$ — contributions to the sinter temperature from evaporation and condensation of water K/s; Q_{pl} and Q_{kr} — contributions to the sinter temperature from the melting and crystallization of the its components, K/s; T_{gas} — air temperature, K; T_{s} — sinter temperature, K; v_z — vertical speed of air passing through sinter, which depends on its length, m/s; FeO — iron oxide; C — carbon; H₂Og — water vapor; O₂ — oxygen; CaCO₃ — calcium carbonate; z — axis with the direction from the surface of the layer downward.

The calculation was done in the computer program Octave. The following initial data were used for the calculation: layer height — 0.5 m; the length of the layer — 30 m; length of preheating part — 5 m; the average velocity of vertical gas flow through the layer is from 0.1 to 0.3 m/s, depending on the path traveled; the speed of the tape, which carries the layer, is 2.9 cm/s; the initial temperature of the layer and gas is 30 °C (below the burners the gas temperature is 1200 °C); the ignition temperature of the coke is 700 °C; the number of steps for the computational grid along the length and height is 30 and 20 respectively; step by time — a quarter of the step along the height of the layer.

Results and conclusions

Figures (1 — 7) show the results of the numerical experiment. Legend in the figures: T_{g} — gas temperature; T_{s} — the temperature of the sinter; $T_{\text{(C+O}_2)}$ — burning start temperature of the coke; O₂ — the oxygen in the air, which comes from the surface of the layer; C — carbon in the layer (burns with the release of heat); FeO — iron oxide in the layer (under the action of O₂ it is oxidized to Fe₂O₃ with the release of heat); CaCO₃ — calcium carbonate in the layer (decomposes with absorption of heat); H₂O is the water in the layer (evaporates with absorption of heat and upon condensation it condenses with release of heat in the lower layers of the sinter); H₂Og — water in the air; the x-axis is the height of the layer in centimeters, where 0 is the surface of the layer; t and d in the titles of the figures — the time and distance traveled along the length of the sinter tape.

In Fig. 2, one can see the decrease in the oxygen concentration during the combustion of coke. It is worth noting that in this paper, a decrease in the rate of all physicochemical reactions in a linear dependence on the concentration of reagents is assumed.

In Fig. 2 and Fig. 3 shows the gradual accumulation of water in the lower layers of the sinter.

This is because in this process the air moving down the layer acts as a carrier of steam.

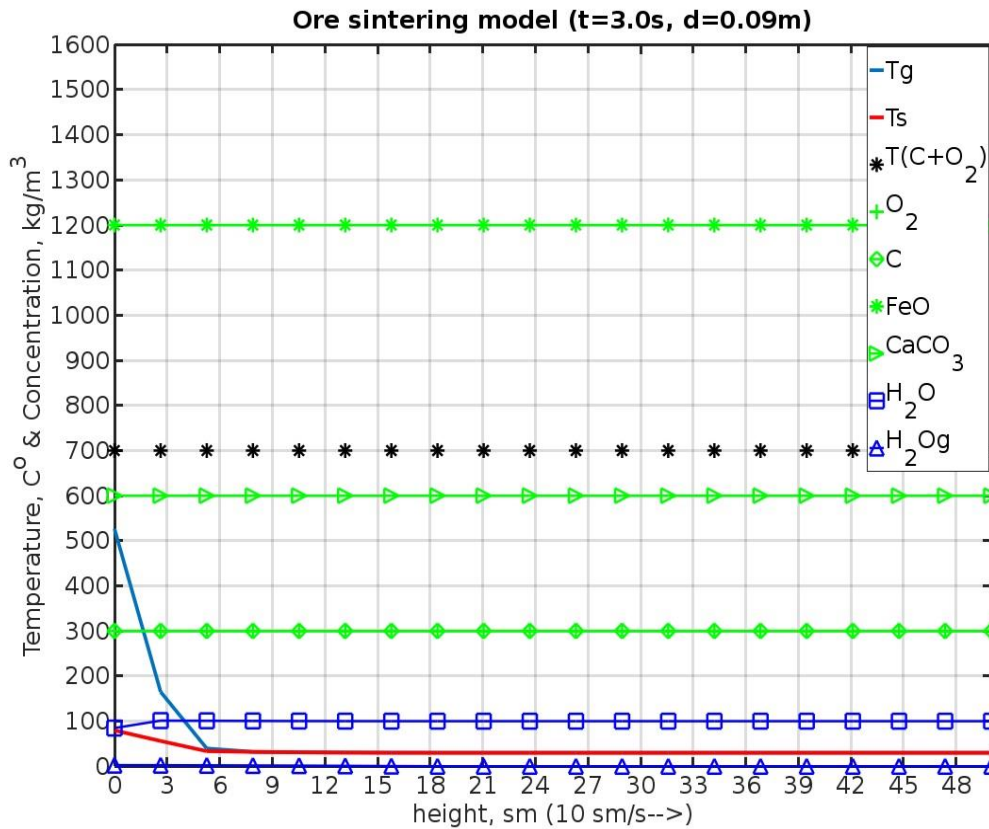


Fig. 1. State of the gas and sinter at the beginning of heating by gas-burners

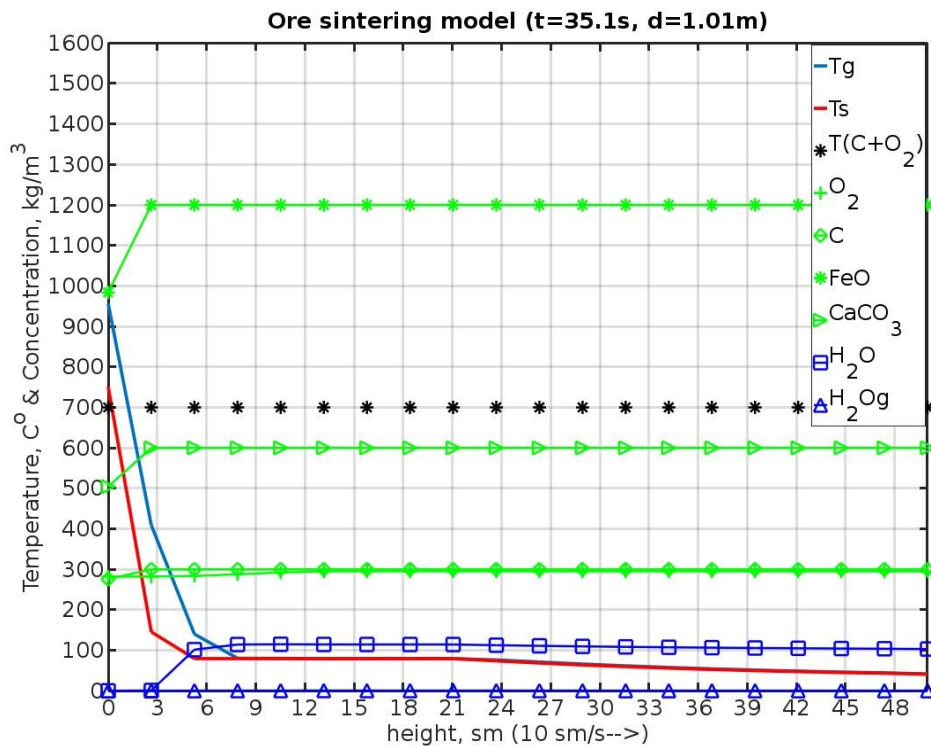


Fig. 2. Start of coke combustion reaction in the sinter (T>700 °C)

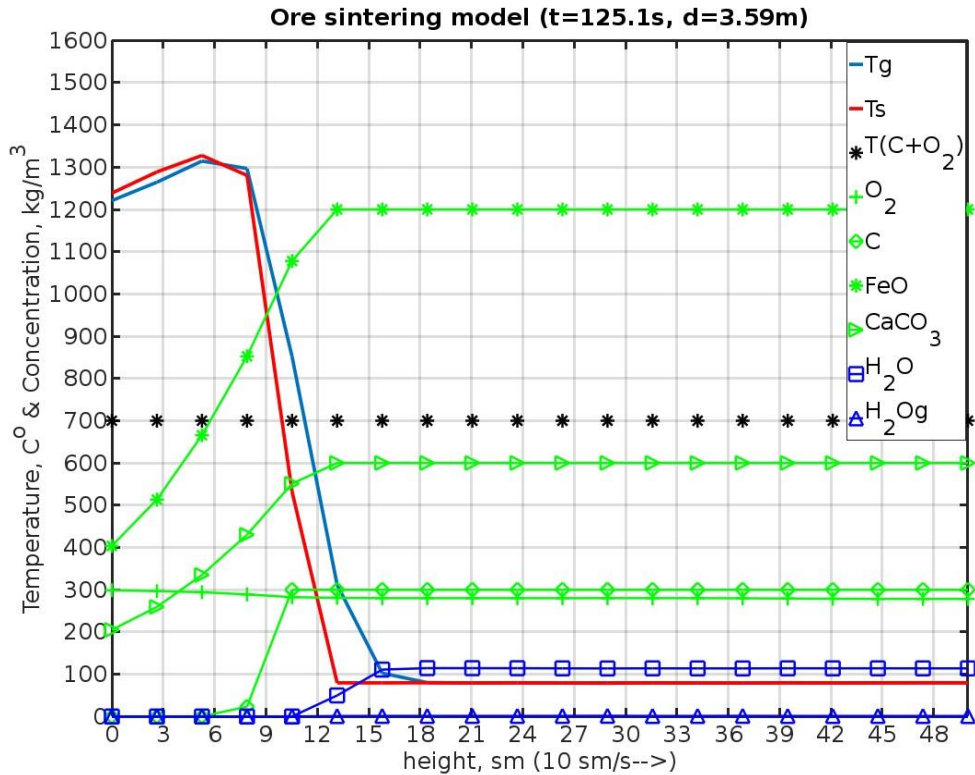


Fig. 3. Temperature increases to 1300 °C in sinter when coke is burned out at a depth of 6 sm

In Fig. 4 the state of a layer's part is shown in the transition to the cooling region of the finished agglomerate, where it is cooled by air with a temperature of about 50 °C.

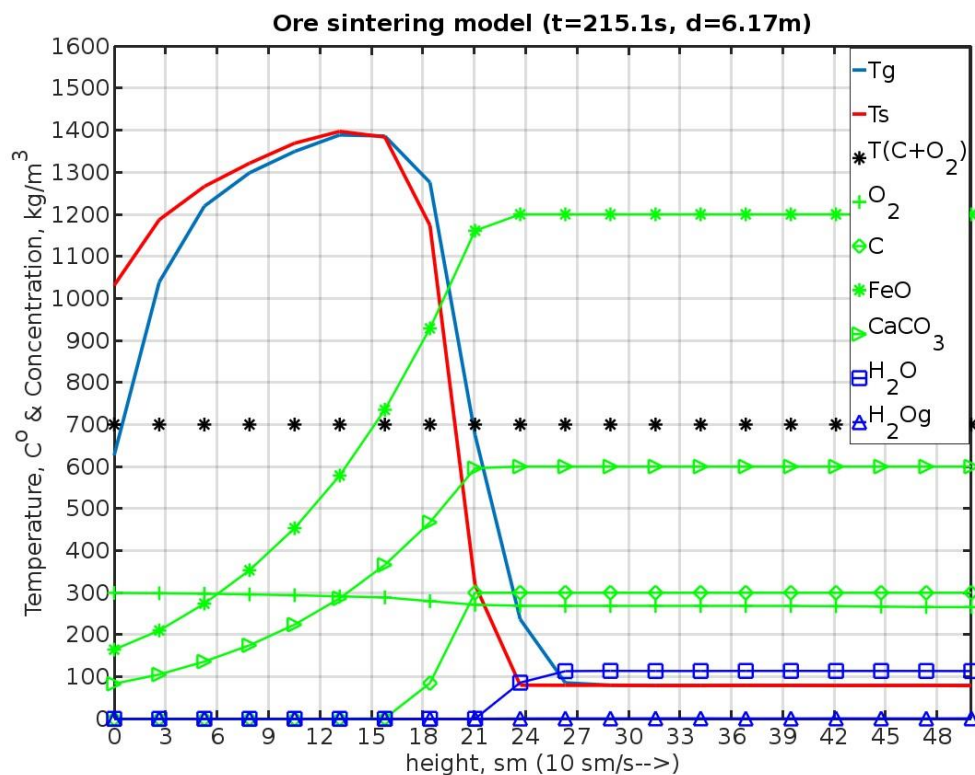


Fig. 4. Transition to cooling area

In Fig. 5-6 with increasing air speed from 0.2 m/s to 0.3 m/s through the layer, you can see a more distinct

difference between the temperature of the layer and the air temperature. Accordingly, the cooling rate of the layer also increases.

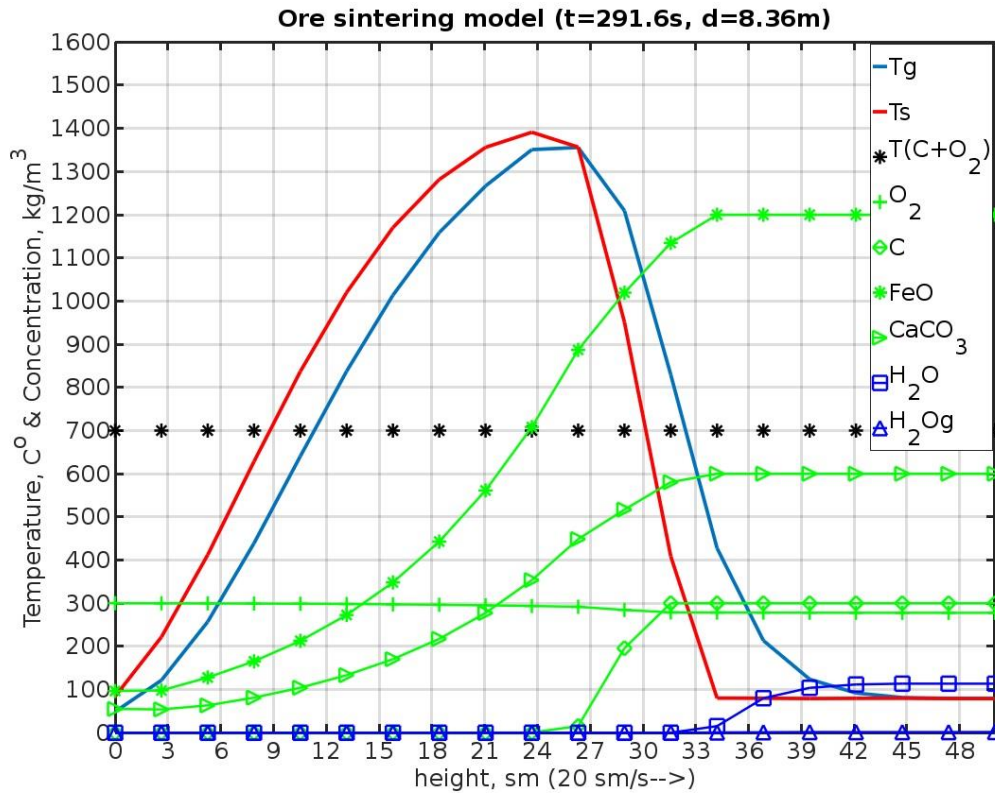


Fig. 5. Speed of air passing through sinter is increased to 0.2 m/s

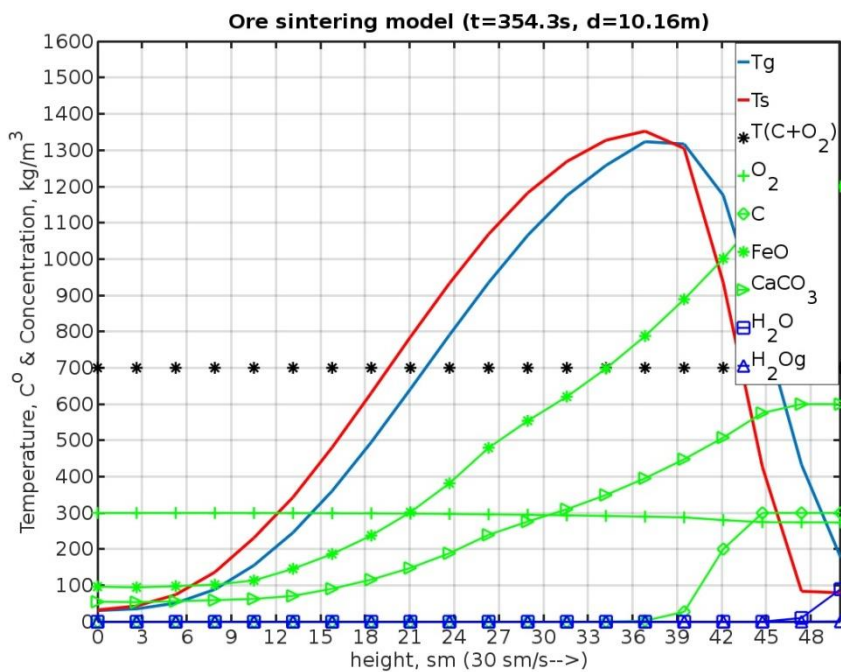


Fig. 6. Increasing of air speed to 0.3 m/s improves cooling further

In Fig. 7, the external isolines correspond to low temperatures, and the internal ones correspond to the temperature around 1400 °C.

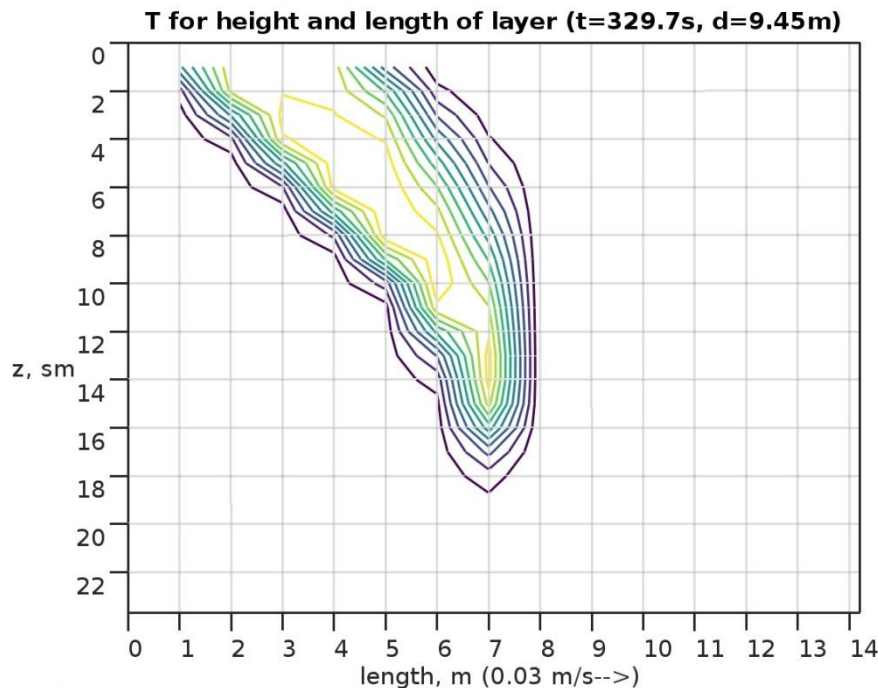


Fig. 7. Distribution of sinter temperature by length and height of layer

The area of coke ignition beneath the burners is clearly visible as well as the expansion of the high temperature region as the layer moves along tape.

An optimization of the metallurgical process is needed to increase its effectiveness. In this work, when carrying out numerical studies using a computer program based on the description of the agglomeration process [1] and the above mathematical model, the temperature distribution in the layer is determined as a function of the gas velocity as it moves vertically through the layer, taking into account the change in the composition of the sinter during the accompanying physical and chemical reactions. The obtained results are consistent with the results and description of the agglomeration process of other researchers [1-2].

The computer model can be adjusted and improved, taking into account other reactions and features of the agglomeration process. For example, in the future it is possible to take into account the heat losses from the walls of the pallets in which the sinter is located, thereby proceeding to a three-dimensional statement of the sintering problem, additionally taking into account the anisotropy over the width of the layer. It is also possible to take into account the features of the lower layer of the sinter (the so-called "bed"), which is usually quite different from the upper layers.

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