

March 2024

NUMERICAL CALCULATION OF THE FLAME SPREADING OVER A METHANE HYDRATE SURFACE

Otabek Nigmatov
nigmatovotabek@gmail.com

Oksana Ismailova
Uzbekistan-Japan Innovation Center of Youth, oismailova56@gmail.com

Follow this and additional works at: <https://cce.researchcommons.org/journal>

 Part of the [Polymer and Organic Materials Commons](#)

Recommended Citation

Nigmatov, Otabek and Ismailova, Oksana (2024) "NUMERICAL CALCULATION OF THE FLAME SPREADING OVER A METHANE HYDRATE SURFACE," *CHEMISTRY AND CHEMICAL ENGINEERING*: Vol. 2023: No. 4, Article 8.

DOI: 10.34920/cce202348

Available at: <https://cce.researchcommons.org/journal/vol2023/iss4/8>

This Article is brought to you for free and open access by Chemistry and Chemical Engineering. It has been accepted for inclusion in CHEMISTRY AND CHEMICAL ENGINEERING by an authorized editor of Chemistry and Chemical Engineering. For more information, please contact zuchra_kadirova@yahoo.com.

NUMERICAL CALCULATION OF THE FLAME SPREADING OVER A METHANE HYDRATE SURFACE

Otabek NIGMATOV^{1,2} (nigmatovotabek@gmail.com)

Oksana ISMAILOVA^{1,2} (oismailova56@gmail.com)

¹Uzbekistan-Japan Innovation Center of Youth, Tashkent, Uzbekistan

²Turin Polytechnic University in Tashkent, Uzbekistan

The Methane Hydrate is expected as an energy source and is being as a medium distance transport means of natural gas alternative of LNG (Liquefied Natural Gas). During the natural gas transportation, fire accidents are concerned. In the present study, the flame spreading over a methane hydrate surface has been studied numerically as a function of hydrate surface temperature, T_s . When $T_s = 173$ K (-100°C), lower than the dissociation temperature ($T_d = 183$ K (-90°C)), the flame spreading speed is around 6.5 mm/s, while the flame spreading speed at $T_s = 193$ K (-80°C), is around 950 mm/s, which is 150 times higher than at $T_s = 173$ K (-100°C). This indicates that the flame spreading speed drastically changed at the dissociation temperature. These results correspond to experimental results. When $T_s > T_d$, the flame spreads gaseous methane/air mixture formed on the hydrate surface and then the flame spreading speed is very fast. When $T_s < T_d$, the flame spreads, dissociating the methane hydrate in front of the leading flame edge by the heat from the flame. Then the dissociation rate determines the flame spreading speed, and it is very slow.

Keywords: , Natural Gas, Numerical Simulation, Flame Propagation, Solid Combustion

ЧИСЛЕННЫЙ РАСЧЕТ РАСПРОСТРАНЕНИЯ ПЛАМЕНИ ПО ПОВЕРХНОСТИ ГИДРАТА МЕТАНА

Otabek NIGMATOV^{1,2} (nigmatovotabek@gmail.com)

Oksana ISMAILOVA^{1,2} (oismailova56@gmail.com)

¹Узбекско-Японский молодежный центр инноваций, Ташкент, Узбекистан

²Туринский политехнический университет в Ташкенте, Ташкент, Узбекистан

Ожидается, что гидрат метана станет источником энергии и средством транспортировки природного газа на средние расстояния, альтернативой СПГ (сжиженному природному газу). При транспортировке природного газа случаются пожары. В настоящей работе численно исследовано распространение пламени по поверхности гидрата метана в зависимости от температуры поверхности гидрата T_s . При $T_s = 173$ K (-100 °C), что ниже температуры диссоциации ($T_d = 183$ K (-90 °C)), скорость распространения пламени составляет около 6,5 мм/с, а скорость распространения пламени при $T_s = 193$ K (-80 °C), составляет около 950 мм/с, что в 150 раз выше, чем при $T_s = 173$ K (-100 °C). Это указывает на то, что скорость распространения пламени резко изменилась при температуре диссоциации. Эти результаты соответствуют экспериментальным результатам. Когда $T_s > T_d$, пламя распространяется газообразную метановоздушную смесь, образовавшуюся на поверхности гидрата, и тогда скорость распространения пламени очень высока. Когда $T_s < T_d$, пламя распространяется, диссоциируя гидрат метана перед передней кромкой пламени за счет тепла от пламени. Тогда скорость диссоциации определяет скорость распространения пламени, а она очень медленная.

Ключевые слова: горение, природный газ, численное моделирование, распространение пламени, горение твердого тела

OLINING METANI GIDRATI USTIDA TARQILISHINI RAQAMLI HISOBI

Otabek NIGMATOV^{1,2} (nigmatovotabek@gmail.com)

Oksana ISMAILOVA^{1,2} (oismailova56@gmail.com)

¹O'zbekiston-Yaponiya yoshlar innovatsiya markazi, Toshkent, O'zbekiston

²Toshkentdagi Turin politexnika universiteti, O'zbekiston

Metan gidrati energiya manbai sifatida kutilmoqda va tabiiy gaz LNG (Suyultirilgan gaz) ga alternativa o'rta masofaga tashish vositasi sifatida xizmat qiladi. Tabiiy gazni tashish paytida yong'in sodir bo'lishi mumkin. Ushbu tadqiqotda metangidrat yuzasiga tarqaladigan olov gidrat sirtining harorati, T_s funksiyasi sifatida son jihatdan o'rganildi. $T_s = 173$ K (-100 °C), dissotsilanish haroratidan ($T_d = 183$ K (-90 °C)) pastroq bo'lganda, olov tarqalish tezligi taxminan 6,5 mm/s, olov tarqalish tezligi $T_s = 193$ K (-80°C), 950 mm/s atrofida, bu $T_s = 173$ K (-100 °C) dan 150 baravar yuqori. Bu dissotsilanish haroratida olov tarqalish tezligi keskin o'zgarganligini ko'rsatadi. Ushbu natijalar eksperimental natijalarga mos keladi. $T_s > T_d$ bo'lganda, olov gidrat yuzasida hosil bo'lgan gazsimon metan/havo aralashmasini tarqatadi va keyin olov tarqalish tezligi juda tez bo'ladi. $T_s < T_d$ bo'lganda, alanga tarqalib, metangidratni olovning issiqligi bilan etakchi alanga chetining oldida dissotsiatsiya qiladi. Keyin dissotsilanish tezligi olovning tarqalish tezligini aniqlaydi va u juda sekin.

Kalit so'zlar: yonish, tabiiy gaz, raqamli simulyatsiya, olovning tarqalishi, qattiq yonish

DOI: 10.34920/cce202348

Introduction

Methane hydrates spread in marine sediments throughout the world, and it has in prospect to be utilized as a new energy source. It is also expected as a transport medium of natural gas alternative to the LNG (Liquified Natural Gas). In this case, an accidental fire during transportation by ships and tank trucks is concerned since the methane hydrate is combustible.

Combustion characteristics have been stud-

ied. A flame over laminar boundary layer over methane hydrate has been done numerically by Kitamura et al. [1] and experimentally by Maruyama et al. [2]. The flame spreading over a methane hydrate surface in a natural convection condition has been experimentally investigated as a function of a surface temperature of a methane hydrate by Yoshioka et al. [3]. Experimental results showed that the flame spreads with around 4 mm/s. When the surface temperature was below the dissociation

temperature, while spreads with around 1,000 mm/s when the surface temperature exceeded the dissociation temperature.

They discussed that in the high-speed flame spreading case of around 1,000 mm/s, the methane hydrate dissociates before the ignition and the flame spreads along the boundary of methane and air layer. On the other hand, in the case of low-speed flame spreading of 4 mm/s, the flame spreads, dissociating the methane hydrate just in front of the leading flame edge due to heat transfer from leading flame edge to the hydrate surface. But this mechanisms of two different flame spreading speed have not been confirmed. Then, the purpose of this study is to elucidate the mechanism of two different flame spreading speed cases mentioned above numerically. The numerical simulation has been done by using Fire Dynamic Simulator [4] (FDS6.7.5).

Numerical Simulation Procedure

The domain for simulation was set following the experimental setup [1] as shown in Figure 1. The three-dimensional space with the grid size of 1mm in 200 mm x 200 mm x 100 mm is set. Initially the space is filled with air of 293 K in the atmospheric pressure. The side and top boundaries are the open boundary.

The bottom boundary is a solid. The methane hydrate with a cylindrical shape with the diameter of 100 mm and 10 mm depth is set at the center of the bottom boundary. In the depth direction, the one-dimensional heat conduction is calculated while another bottom wall was set as an adiabatic. A block of 10 mm square and 3 mm height is set as an ignitor at the center. The surface temperature of this block is set at an arbitrary temperature. This is equivalent to the pilot flame for the ignition in experiments. When the ignition is calculated, the temperature of the bottom wall of the block is set

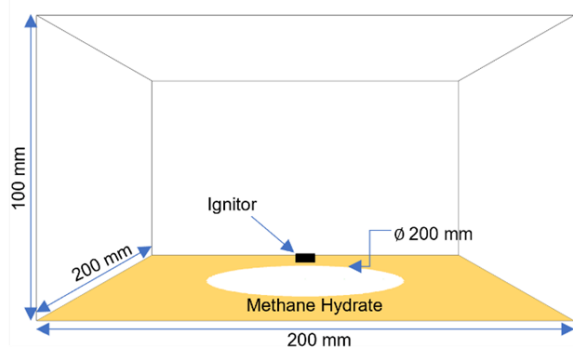
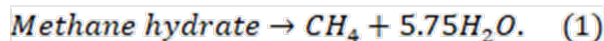


Figure 1. Calculation domain.

as 1273 K while the top and side walls are at 293 K for the low-speed flame spreading case, however for the high speed-flame temperature of bottom and side walls are set as 1473 K, since in the high-speed flame spreading case the methane release rate is higher than in the case of low-speed flame spreading and the hot walls of the block require longer time to heat up to the ignition temperature, the temperature of the block and hot temperature walls are preferred. Moreover, for two different cases, the height of the block was set up in different positions. For high-speed flame spreading case 14 mm above the surface of methane hydrate and for low-speed flame spreading case 8 mm above the surface of methane hydrate.

In numerical calculation, governing equations, continuity equation, momentum equation, energy conservation equation, species conservation equation with chemical reaction models mentioned below were solved by the FDS [5]. In the present study, two chemical reactions are included. One is a dissociation of methane hydrate, and the other is a methane and air combustion.

The dissociation of methane hydrate is modeled as,



Here 5.75 is a theoretical ratio of water and methane in a methane hydrate. In realistic conditions, this value is larger, however in this study we set it as a theoretical value.

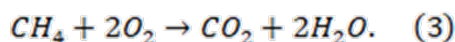
The dissociation rate is expressed modifying the Pyrolysis mode in the FDS as,

$$r_{ij} = A_{ij} Y_{i,j}^{n_{s,ij}} \exp\left(\frac{-E_{ij}}{RT_s}\right), \quad (2)$$

Where A_{ij} is a pre-exponential factor, $Y_{i,j}$ is a mass fraction of species i , $n_{s,ij}$ is the reaction order, E_{ij} is an activation energy, R is an universal gas constant and T_s is a methane hydrate surface temperature. Here the subscript i represents the species i and j the reaction j . There are three species, methane hydrate, methane, and water. The values for the pre-exponential factor and the activation energy are $5.44 \times 10^{21} \text{ s}^{-1}$ and $8.42 \times 10^4 \text{ J/mol}$ respectively. These values are obtained from the direct measurement of decomposition rates of pure methane hydrate at the ambient pressure of 0.1 MPa experimentally by Laura et al., [6]. However, the Pyrolysis model of FDS, [5] does not show similar trend of dissociation, so approximation was done.

The methane and air combustion are mod-

eled by the one-step overall reaction as following,



The combustion is modeled with using of auto ignition temperature by FDS [5]. The auto ignition temperature is the temperature at which combustion starts.

Numerical Calculations have been done two cases; One is the low-speed flame spreading case when initial methane hydrate temperature is 173 K which is lower than methane hydrate dissociation temperature, and the second high-speed flame spreading case when the hydrate temperature is 193 K which is higher than the methane hydrate dissociation temperature.

Results and Discussion

High-speed flame spreading ($T_s = 193$ K)

Figures 2-4 show the results at $T_s = 193$ K. T_s is higher than the dissociation temperature and the high-speed flame spreading was observed in the experiment [3].

Figure 2 shows the time variation in the mass fraction of methane. At $t = 0.0$ s, the space is filled with only air and no methane gas. The hydrate starts to dissociate uniformly over the methane hydrate surface because T_s is higher than the dissociation temperature and the methane gas is released uniformly over a methane hydrate surface as shown in $t = 0.05$ s. The methane region almost reaches the block at $t = 0.1$ s. After that, the top location of methane is located just below the block.

The variation in the temperature profile

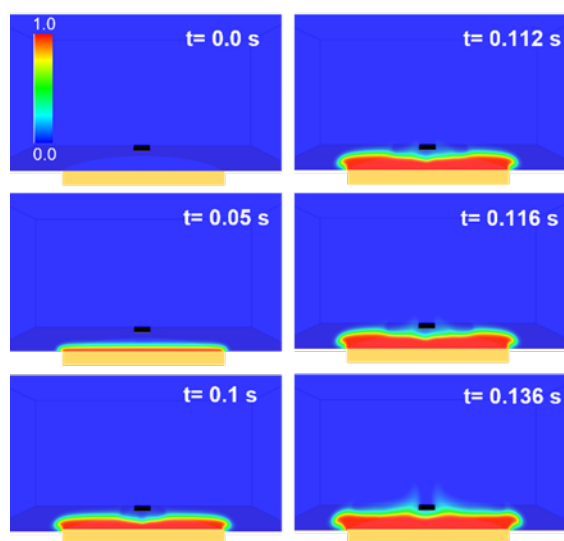


Figure 2. Methane mass fraction for high-speed flame spreading

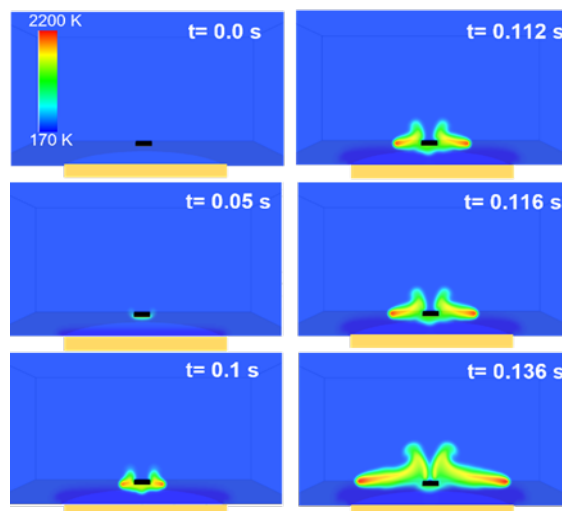


Figure 3. Temperature for high-speed flame spreading.

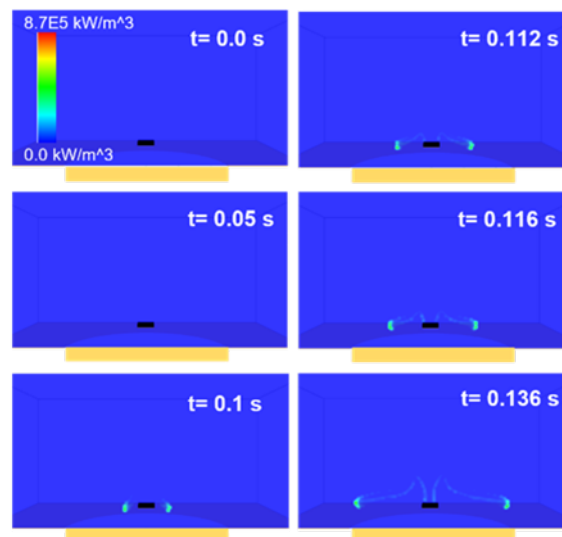


Figure 4. Heat release rate for high-speed flame spreading.

with time is shown in Fig. 3. At $t = 0.0$ s, all area of the space is the ambient temperature (293 K). At $t = 0.05$ s, slight increase in temperature is observed in the region which is adjacent to the high temperature block. At $t = 0.1$ s, significant temperature increase is calculated. The high temperature region moves radially with time. At the same time, the high temperature region moves upward direction due to the gravity effect.

Figure 4 shows the heat release rate. At $t = 0.0$ and $t = 0.05$ s, no high heat release rate region is observed. At $t = 0.1$ s, significantly high heat release rate region appears near the high temperature block and the region moves radially.

These results indicate that the ignition occurs between $t = 0.05$ s and 0.1 s. At $t = 0.05$ s, the temperature increases slightly but no high heat release rate region appears. This indicates the air

around the high temperature block is heated by the heat from the block but not yet start the combustion. At $t = 0.1$ s, the temperature increase is very significant, and the high heat release rate region appears which means the flame is already formed. After that, high heat release rate region, which is considered to be the leading flame edge moves radially, that is a flame spreading. As shown in Fig. 4, the heat release rate region moves radially with almost constant speed. Then, the flame spreading speed is estimated as 950 mm/s from a movement speed of the high heat release rate region, which is nearly the same as the experimental one.

Low-speed flame spreading case ($T_s = 173$ K)

Figures 5-7 show the results at $T_s = 173$ K. T_s is lower than the dissociation temperature and the low-speed flame spreading was observed in the experiment [3].

Figure 5 shows the time variation in the methane mass fraction. At $t = 0.0$ and 1.1 s, no methane is observed, although the uniform methane layer was already observed at $t = 0.05$ s at $T_s = 193$ K. At $t = 2.0$ s, small amount of methane appears between the methane hydrate surface and the high temperature block. The amount of methane increases gradually with time however it is very slow compared to the case in $T_s = 193$ K. Results show methane release was observed locally which is different compared to the case at $T_s = 193$ K.

Figure 6 shows the variation in temperature with time. The temperature increases around the high temperature block at $t = 1.1$ s and the high temperature region spread in radial and upward directions. Figure 7 shows the heat release rate. At $t = 1.1$ s, the high heat release region appears near the methane hydrate surface just below the high temperature block. It clearly states that the dissociation starts locally in the region with high heat transfer from the block. After the formation of the flame, the dissociation occurs by the heat from the leading flame edge and the high heat release rate region moves radial direction with the dissociation of methane hydrate just in front of the flame leading edge which is the radial flame spreading. Then the speed of flame spreading is estimated as 6.5 mm/s this is the same order of magnitude of that in experiment [3]. In addition, it is interesting to note that the high heat release rate region is observed in the vertical direction. It indicates that the flame is formed in a vertical direction as well. It corresponds to the experimental result [3]. The numeri-

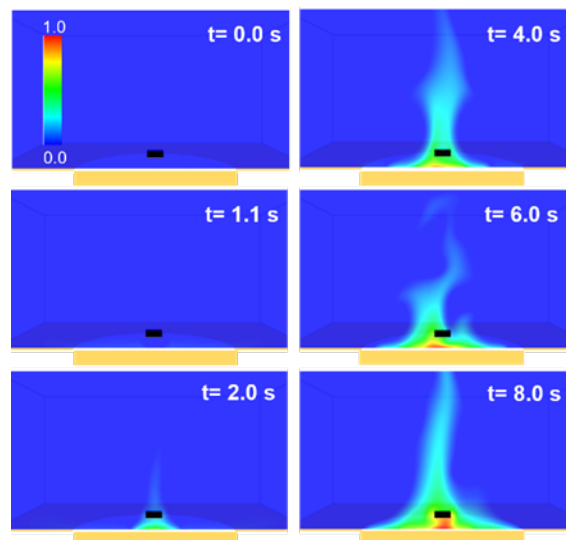


Figure 5. Methane mass fraction for low-speed flame spreading

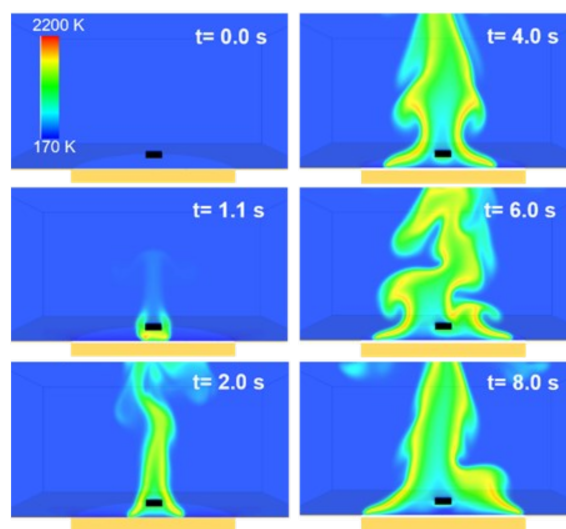


Figure 6. Temperature for low-speed flame spreading

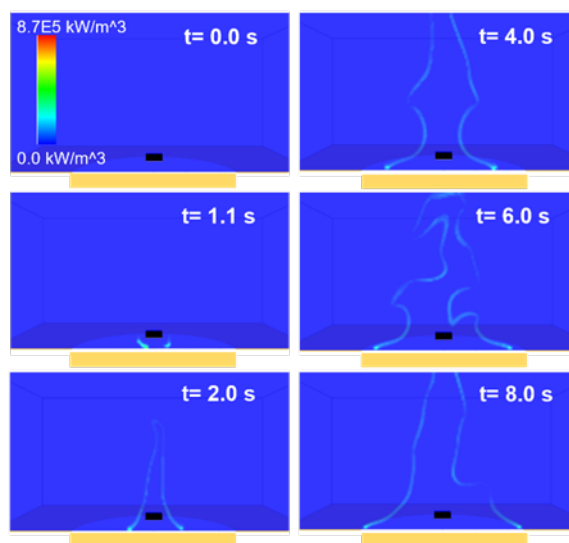


Figure 7. Heat release rate for low-speed flame spreading

cal result shows some unstable motion in a vertical direction which is shown in Fig.6. The experimental result shows similar instability. This instability is due to the Kelvin-Helmholtz instability between high speed hot burnt gas flow and still ambient temperature of air.

Flame spreading speed

Figure 8 shows the comparison of flame spreading speed of numerical and experimental ones. The result show that the numerical results well fit with experimental ones [3]. It indicates that the flame spreading speed is very low when the hydrate surface temperature is below the dissociation temperature while it increases around factor of 150 when the hydrate surface temperature exceeds the hydrate dissociation temperature.

Flame spreading mechanism

Two kinds of flame-spreading numerically calculated. First is high-speed flame spreading of $T_s = 193$ K. In this case, the methane hydrate starts to release into the ambient air producing methane/air mixing layer. After this mixing layer reaches the high temperature block, the ignition occurs, and flame spreads along the mixing layer in a radial direction. Second is the low-speed flame spreading case of $T_s = 173$ K. In this case, the surface temperature is below the dissociation temperature and then the dissociation cannot occur by the ambient air temperature. As a result, no uniform methane release over a methane hydrate surface occurs different from the case in $T_s = 193$ K. The methane hydrate surface near the block starts to dissociate by the heat transferred from the block locally and the combustion starts. When the flame is formed, high heat flux from the leading flame edge to the methane hydrate sur-

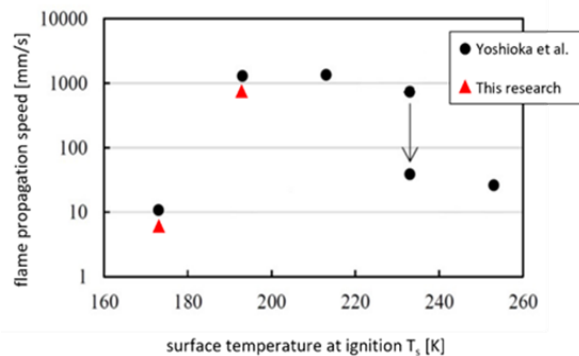


Figure 8: Flame spreading speed with surface temperature.

face dissociates the methane hydrate just in front of the leading flame edge. Thus, the flame spreading speed is determined by the dissociation rate just in front of the flame leading edge.

Conclusion

Two cases of flame spreading over an axisymmetric methane hydrate surface have been calculated numerically: high-speed flame spreading and low-speed flame spreading. The result in the high-speed flame spreading indicates that uniform dissociation of methane hydrate makes a uniform contact surface of methane and air, and the flame spreads along the contact surface at around 950 mm/s which is near to experimental result of flame spreading in high-speed case. When the surface temperature of methane hydrate, T_s , was lower than the dissociation temperature, the flame spread slowly at around 6.5 mm/s, which corresponds to the experimental result. In this case, the flame spreads, dissociating the methane hydrate in front of the leading flame edge. It indicates that the flame spreading speed is determined by the dissociation rate of methane hydrate.

REFERENCES

1. Kitamura Y., Nakajo K., Ueda T. Numerical calculation of a diffusion flame formed in the laminar boundary layer over methane-hydrate. *Proc. 4th Int. Conf. on Gas Hydrate*, 2002, 4, 1055–1058.
2. Y. Maruyama, M. J. Fuse, T. Yokomori, R. Ohmura, S. Watanabe, T. Iwasaki, W. Iwabuchi, and T. Ueda, Experimental investigation of flame spreading over pure methane hydrate in a laminar boundary layer. *Proc. Combust. Inst.*, 2013, 34, 2131–2138.
3. Yoshioka T., Suemitsu M., Yokomori T., Ohmura R., Ueda T. Me Flame propagation over a methane hydrate with surface temperature variation in a natural convective flow field. *Engineering Letters*, 2015, 1, No.15-00370. DOI: 10.1299/mel.15-00370
4. FDS-SMV, available at <https://pages.nist.gov/fds-smv/>
5. Kevin McGrattan K., Simo Hostikka S., Randall McDermott R., Jason Floyd J., Weinschenk C., Overholt K. *Fire Dynamics Simulator Technical Reference Guide Volume 1: Mathematical Model*, NIST Special Publication 1018-1, Sixth Edition, 2020. 173.
6. Stern L.A., Cirone S., Kirkby S.H., Durham W.B. Anomalous preservation of pure methane hydrate at 1 atm. *The Journal of Physical Chemistry B*, 2001, 105/9, 1756-1762.