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<sup>1\*</sup>Shalymova A.E.,

Master student, ORCID ID: 0009-0007-3888-6686, e-mail: shalymova.aigerim@gmail.com

PhD, Professor, ORCID ID: 0000-0002-1937-8615, e-mail: alibek.issakhov@gmail.com

<sup>1</sup>Kazakh British Technical University, 050000, Almaty, Kazakhstan

## NUMERICAL MODELING OF OIL AND PETROLEUM PRODUCTS DISTRIBUTION IN CASE OF AN EMERGENCY SPILL ON THE WATER SURFACE

#### Abstract

Water pollution is an urgent problem today. The amount of water pollution with petroleum products is growing as oil production increases, oil transportation becomes globalized, and new fields are put into operation. This has a detrimental effect on the ecosystem. The aim of the work is to numerically simulate the spread of oil product on the water surface, which can help improve the efficiency of planning and operational management of measures for the localization and elimination of emergency spills. Different emission rates of the pollutant (gasoline) were considered in order to investigate how the pollution area varies for each speed. To model this problem, the Navier-Stokes equations for an incompressible fluid are used as a mathematical model. The numerical solution of the Navier-Stokes equations was achieved using a SIMPLE algorithm. A test problem was performed to verify the numerical method and the mathematical model. The calculation results were compared with the result of the experiment and showed an excellent match.

Key words: mathematical modelling, oil spill, water pollution.

#### Introduction

Water is the basis for human life and health and everyday functions. We have a lot of it on Earth. Nevertheless, water pollution is a pervasive problem with several sources consisting of industrial unwanted emissions, agriculture, and waste from urban lives. [1] The foremost hazard this is harmful petroleum products, which can have very bad effect on ecosystems, human health and economy. The instances of water poisoning can occur when petroleum products, such as gasoline, diesel, lubricants, and crude oil are dumped either intentionally or accidentally into a water body. Among the most characteristic types of pollution by petroleum in the water bodies is the oil spills.

Oil spills are a relatively common incident however, we may tend to underestimate how often they happen from diverse sources. Along with oil production and transportation, and especially during oil field operations, the annual number of oil spills continues to increase. Every year, around the world, oil spills happen up to 70,000 times. While most of them are relatively small in scale, take fuelling deep-sea ships, for example. On the other hand, when oil spills occur on the coasts, mangroves, and bogs which are very sensitive, they are deadly with long-lasting effects. Oil spills of larger amounts can cause ecological catastrophe with big consequences for our environment and economy. Therefore, we should take measures for oil spill prevention. This type of disaster is usually caused by pipeline cussing, crude oil spills from super tankers and booms occurring during drilling operations. These stories, which eventually occur in profusion and enormous volumes, have terrible and multiple effects simultaneously on the ecosystems and economies. Oil spillage potentially takes place throughout the course of its extraction, ranging from drilling to transportation and processing. The main danger, that occurs in the process, is of planetary character. There is a wide variety of organisms that thrive in these spills in marine environments whether aquatic, land-based, or airborne. The same serves as the blocker of sunlight for the water with a reduction in the oxygen content in the water. On birds and mammals, the oil harms feather and fur, but it is not destructive to the structure which does not fall off (shedding), thus animals can die from hypothermia. The fish early in life are more sensitive to the oil effects as compared to adult fish thus in instances of significant exposure to a huge number of fish the initial stage of death occurs. Another danger is oil polluting the food chain it can be fatal to many species recovering the habitats even after the oil spill is eliminated is possible.

There are many studies which speak about this problem. [2] presents the finite element model and the COMSOL multi-physics software for 1st order differential leak detection in crude oil pipelines directly. The work [3, 4] encompasses a detailed and comprehensive mathematical model of the river pollution arising from the pipeline rupture. They research the role of different water body's characteristics as well how they affect hydrocarbons movement in the water system.

The model of the movement of an oil spill along the Bosphorus Strait, which is a very important port on Turkey, is also a responsibility of them [5]. The model serves as an informative illustration of the movement of the oil spill which reveals that in just four hours the oil spill can reach both banks of the street already, implying emergency response should be implemented after the accident about the oil spill. In [6] ADIOS and GNOME models are among the tools that AWI uses to simulate oil spill dynamics in New York Bay with the intention of assessing its environmental consequences. This part concentrates on the behaviour of oils of various types under different circumstances, at the same time highlighting the significance of environmental features, for example, wind, and currents in shaping spill paths and decomposition processes. The experiment says the light oils like gasoline are evaporating swiftly, the risk of contamination is less, and heavy oils are not. In [7] is a paper that shows how oil spill modelling can be done using adjoin-methods in an attempt to find the source of emissions and the time of their entry. It sorts out the advection-diffusion equation to convey how oil spill's function and offers a brand-new technique for locating the pollution origin by numerical simulation. The effectiveness of this method comes out of examples as shown in the case studies of the Vietnamese coast. [8] uses geospatial hydrodynamic and oil spill models to investigate the environmental effects of the oil spill at Tramandai Beach. The simulation takes place by simulating a spill and following wind and currents contributes to the oil movements and dispersion. Data are confirming that the oil hit the shoreline in 10 hours, where wind and currents were responsible for the right timing and destination of the spill ultimately.

Some studies that mean prediction of oil spills and assessment of risks are conducted. In [9] discusses the hazard of spilling oil into the Bohai sea focusing on the risk of shipping and offshore drilling catastrophic disasters. Coinciding spatially and historically important data, the research detects the areas of high spill risks and gives a probabilistic model for assessing their spill probabilities. Based on this detection, seven high-risk locations have been shown as strategic places where spill response equipment might be stored. In [10] aims to precisely reproduce the spread of oil spills as well as processes such as surface spreading, transport by advection, turbulent diffusion, evaporation and interaction with shorelines. It is completed with the 3-D hydrodynamics and a wave model in order to increase the hydro-environmental simulation precision. The case study, designed to imitate an oil leak in Dalian, is bound to portray the power of the model to predict the dispersion and fate of the oil. Considering [11] the model performing with local hydrological data and taking into consideration seasonal variations, the model successfully predicted the estimated movement of contaminants from various sources like Chernaya River and Gollandiya Bay. The season analysis of pollutant diffusion reveals that the local water circulation patterns and the wind conditions basically determine the fluctuations of pollutant spread. In [12], they are deepened taking advantage of 2D and 3D transferdiffusion equations, estimating the behaviour of the pollutants and calculating risk level.

In [13] showcased the role of mathematical models as a primary tool in the management of environmental disasters, such as an oil spill, through the illustration of their efficiency by predicting pollutant behaviour and provision of necessary information for mitigation and clean-up activities. Many authors have written papers to add to the existing knowledge base of oil spill behaviour in marine ecological systems and its effects. In [14] provide detailed information on how oil spills affect the flow paths and oil distribution in the immediate spill area and nearby flow domains, which in turn improve the understanding of the dynamics of oil spills and are an avenue for the development of the management or mitigation of oil-in-water spills. In [15], to construct a mathematical model that is based on the principle of linking ordinary differential equations to identify and predict the consequences of exposure to oil pollutants in the marine environment, the MATLAB software was used for the solution [16]. This work was concentrated on the creation of a coded model for oil spill drift modelling in coastal waters. In [17] researched the spreading of oil pollutants throughout the Rioni River and Black Sea. In [18] the dynamic when oil spills under different scenarios such as continuous low-intensity releases as well as high-intensity short-term accidents have been presented in detail with regard to oil emission at the sea surface and seabed. In [19], this case involved Deepwater Horizon oil leak modeling which included hydrodynamic, wave, and weather conditions in order to simulate oil spread. In [20] carried out the oil spill dynamics with the MOHID software used and assessed the São Sebastião area, which is thought to be the most important marine terminal in Brazil. In [21] constructed a computer model to model the temporal and spatial alterations of pollutants after water pollution incidents. In [22] examined the pollution in the Ganges River, especially in the urbanized areas of cities including Kanpur and Varanasi.

#### Main provisions

This study focuses on the mathematical and computational modelling of oil and petroleum product dispersion in the event of accidental spills on water surfaces. The primary aim of this research is to conduct numerical simulations of petroleum product spread on water surfaces, with the objective of enhancing the efficiency of planning and operational management of measures for the containment and remediation of spill incidents.

To achieve this objective, the Navier-Stokes equations were employed for modelling purposes. These equations are fundamental in fluid dynamics and are particularly suitable for simulating the behaviour of oil spills on water bodies. Furthermore, the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) method was utilized for numerical solution, chosen for its effectiveness in addressing the complexities associated with fluid flow problems.

The findings of the simulations demonstrate a direct correlation between the extent of contamination and the rate of discharge. Specifically, an increase in discharge velocity by a factor of two resulted in a 17% increase in contamination area, while a decrease in velocity by the same factor led to a 12% reduction in contamination area. These results highlight the significance of considering discharge velocity as a critical parameter in the planning and execution of strategies for the localization and mitigation of spill incidents.

## **Research** area

We are considering the area where the Ural River flows into the Caspian Sea. The Ural is a river that has its source in the west of Russia and runs through different regions, including those of the countries, Russia, and Kazakhstan. The length of the Ural River is 2,428 km and its watershed has 231 land area. The amount of annual runoff is around 12,6  $km^3$ , and the water at the mouth is 400  $m^3/s$ .

The river gets back 94% of water resources from the melting of snow mass in the mountains and in lower elevations and 6% supply comes from groundwater and from underground water sources. The river's water resources are used for irrigation of the large city people of which the forming of the reservoirs along the Urals River has been done as well as communications of water utilities and

sewage treatment plants have been created to be seated on the dams. In the regions of oil and gas production, chemical raw materials processing, including competitive industries arise at the Ural River shores.



Figure 1 – Location of the research area.

## **Materials and Methods**

Mathematical model

The mathematical model contains a non-stationary equation of continuity, momentum, heat transfer, and concentration transfer.

Continuity equation:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

Momentum equations:

$$\frac{\partial u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = \frac{\partial \left(-\rho \overline{u'_i u'_j}\right)}{\partial x_j} - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right)$$
(2)

Heat transfer equation:

$$\frac{\partial T}{\partial t} + \frac{\partial (\rho u_j T)}{\partial x_j} = \frac{\partial (-\rho u_j' T')}{\partial x_j} + \frac{\partial}{\partial x_j} \left( D \frac{\partial T}{\partial x_j} \right)$$
(3)

Concentration transfer equation:

$$\frac{\partial C}{\partial t} + \frac{\partial (\rho u_j C)}{\partial x_j} = \frac{\partial (-\rho u_j' C')}{\partial x_j} + \frac{\partial}{\partial x_j} \left( D \frac{\partial C}{\partial x_j} \right)$$
(4)

here,  $u_i$  – velocity,  $\mu$  – viscosity,  $\rho$  is the density of the liquid, and P is the fluid pressure, T – temperature of the liquid, D – the diffusion coefficient,  $\overline{u'_i u'_j}$  – turbulent fluxes of velocity,  $\overline{u'_j T}$ ,  $\overline{u'_j C}$  – turbulent fluxes of heat and concentration of pollutant (benzene).

The given set of equations is a representation of a physical system in the Cartesian coordinate system  $x_i$ , where i take the values 1, 2, and 3. The system consists of 3 velocity components, namely  $u_i$ .

#### Numerical modelling

Along the Zhaiyk River in the proximity of Atyrau city where the pollution is going to take place 2D models of the pollution made it possible to model the processes. Notably, even the most powerful computing clusters cannot feasibly execute full 3D modelling for many real-world scenarios. The area which is modeled with the aid of the 2D model can be seen in Figure 1. Using a two-dimensional model allows us to coarsely evaluate the profile of flow fields with temperature and pollutants as well as chemical reactions directed in different directions.

The SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm was used as a numerical algorithm. Complete SIMPLE algorithm includes following steps:

1. Guess the pressure field  $p^*$  and solve the momentum equations to obtain  $u^{**}$ ,  $v^{**}$ .

$$\frac{u^{**} - u^n}{\Delta t} = -\frac{1}{\rho} \frac{\partial p^*}{\partial x} + L_1 \Rightarrow u^{**} = u^n + \Delta t \left( -\frac{1}{\rho} \frac{\partial p^*}{\partial x} + L_1 \right)$$
$$\frac{v^{**} - v^n}{\Delta t} = -\frac{1}{\rho} \frac{\partial p^*}{\partial y} + L_2 \Rightarrow v^{**} = v^n + \Delta t \left( -\frac{1}{\rho} \frac{\partial p^*}{\partial y} + L_2 \right)$$

2. Solve the p' equation by substitute into the continuity equation and we get the Poisson equation

$$\frac{u^{n+1} - u^{**}}{\Delta t} = -\frac{1}{\rho} \frac{\partial p'}{\partial x} \Rightarrow u^{n+1} = u^{**} - \frac{\Delta t}{\rho} \frac{\partial p'}{\partial x}$$
$$\frac{v^{n+1} - v^{**}}{\Delta t} = -\frac{1}{\rho} \frac{\partial p'}{\partial y} \Rightarrow v^{n+1} = v^{**} - \frac{\Delta t}{\rho} \frac{\partial p'}{\partial y}$$
$$\frac{\partial^2 p'}{\partial x^2} + \frac{\partial^2 p'}{\partial y^2} = \frac{\rho}{\Delta t} \left( \frac{\partial u^{**}}{\partial x} + \frac{\partial v^{**}}{\partial y} \right)$$

3. Correct pressure field  $p = p' + p^*$ .

4. Correct velocity field  $u = u' + u^*$ ;  $v = v' + v^*$ .

This algorithm is widely used to solve Navier-Stokes equations.

#### **Model verification**

To test the mathematical model and numerical algorithm, a test problem was performed. The problem was to develop an open channel and lateral tap model from [23]. The reactor comprised two channels and is shown in the Figure 2. It was assumed that the diameter of the pipe was 5 mm which is equal to D. In addition, the vertical channel was positioned exactly on the X-axis in the middle at 100 mm (20D) from the beginning of the horizontal channel. The width of the main section and the height of the pipe were 120 mm (24D), and its length was 505 mm (101D). At first, the temperature of the warm water was 25°C, and the temperature of the hot water was 81°C. Figure 2 shows a laminar jet that enters the channel in the frontal direction. The conditions for the pipe and crossflow were set using 2 distinct target velocities. For example, the velocity in the horizontal duct was set at 2,005 m/s, and in the vertical duct - 11,969 m/s. To model this problem numerically, the viscosity of the water was set to 0,001003 kg  $m^2$ /s and the density to 998,2 kg/m<sup>3</sup>.



Figure 2 – Geometry and boundary conditions of the test problem.

$$Q = \frac{T - T_{\infty}}{T_j - T_{\infty}}$$
$$U = \frac{U - U_{\infty}}{U_{max} - U_{\infty}}$$

here,  $T_{\infty}$  represents the ambient temperature,  $T_j$  denotes the pipe temperature, Velocity U indicates the velocity across the X-axis, and  $U_{max}$  signifies the highest value of the velocity across the X-axis.

Figure 3 (p. 145) represents a comparison of experimental data with numerical solutions from different grid sizes. To be more precise, the grid sizes of 2,5 mm, 3 mm, and 4 mm were used. It can be seen from the figure that the results with a grid size of 4 mm where 4034 nodes and 3848 elements coincide well with the experimental data. To completely match the algorithm with a test problem, the numerical results were compared with empirical results [24], as well as with computational results of other researchers [23] for different cross-section dimensions (X/D = 2, 4, 6, 8, 10).

Figure 4 (p. 146) represents dimensionless temperature profiles in the vertical direction. The outcomes of the numerical modeling exhibit favourable alignment with the empirical findings. It is evident from the collected data that the numerical results reasonably correspond to the experimental data. For the numerical solution of this problem, the SST k-w turbulent model was used.

Numerical results of pollution of the Caspian Sea

A computational framework was designed to numerically model the concentration transfer of oil product (benzene) in Zhaiyk River and then in the Caspian Sea. Figure 1 represents the satellite image of the area we are concerned, while Figure 4 shows the geometry of the region. The computational area includes a span of 6500000 x-axis and 4082500 y-axis, respectively. This equals 1062500 m x 648100 m. The area of the research area was 6886062500  $m^2$ . The casework included 3 ways of pollutant liberation with varied rate values. The computational grid of 466852 tetrahedral elements 10 m per cell, evenly spread over the total river region and sea surface extending toward 200 m constructed the design. Furthermore, the grid was refined in the direction of the product out flux partition along with the element size of 0,1 m for this particular zone. This refinement was thereby done to improve the precision of the mathematically based outcomes.



Figure 3 – Temperature profiles for different mesh sizes.

## **Results and Discussion**

It was supposed that some spill of oil products into Zhaiyk River had to be over during the emergency refinery situation. Then the oil product spreads along the river and all this falls into the Caspian Sea, where the Zhaiyk River flows. For an accurate forecast of the spread of an oil slick, the real velocity of the river and wind are taken into account. According to Figure 5 at inlet 1, the average wind velocity over the sea is accounted for, at 5,49 m/s. At inlet 2, the velocity of the Ural River is considered, at 0,3 m/s. At inlet 3, the emission rate of the pollutant is taken into account, at 0,03 m/s. According to Table 1, the pollution area was 1126143218,94  $m^2$  as the pollutant level was 0,03 m/s. Nevertheless, the emission factor of 0,06 m/s got the water of 1318207280,65  $m^2$  polluted. Accordingly, when emission intensity is 0,015 m/s, the affected area is 987727620,15  $m^2$ . In fact, slashing the emission rate in half would lead to a 12,3% area reduction, and if we doubled the emission rate of the pollution area on the emission rate.



Figure 4 – Vertical profiles of temperature at the indicated points.



Figure 5 – Geometry of the main problem

| u         | the area of contamination |
|-----------|---------------------------|
| 0,03 m/s  | 1 126 143 218,94 $m^2$    |
| 0,06 m/s  | 1 318 207 280,65 $m^2$    |
| 0,015 m/s | 987 727 620,15 $m^2$      |

## Table 1 – The area of the pollution zone at different rates of release of the pollutant



Figure 6 – Dependence of the pollution area on the emission rate.



Figure 7 – Distribution of the contaminant for velocity u= 0.03 m/s



Figure 8 – Distribution of the contaminant for velocity u= 0,06 m/s



Figure 9 – Distribution of the contaminant for velocity u= 0,015 m/s

## Conclusion

The study aims to develop a model describing the spreading of oil products and petroleum in case of an emergency release on the water reservoir, taking into account wind velocity and water streaming velocity. The results of numerical modeling showed that the emissions directly influenced the pollution area. Considering 3 different emission rates (u=0.03 m/s, u=0.06 m/s, u=0.015 m/s) from Table 1, it seems an increment in the emission rate will result in a larger pollution area, but an

emission rate reduction leads to a pollution area decrease. Figures 7, 8, and 9 depict the concentration of the maximum allowable amount of gasoline in 24 hours. This demonstrates the need to slow down and regulate the rate of release in case of overflowing of the spilled liquid. Doing so reduces the pollution area and lowers the negative impact on the environment. But in addition to these components, there are some others, for example, wind velocity and rivers are the determining factors of the spread of pollution. Consequently, a modeling for the transportation of oil and petroleum products shows not only the importance for predicting the spread of accidental spills, but also calls for the development of strategies and measures to prevent and respond to such spills with an aim of minimizing the negative impact.

Beyond, this research has provided opportunities for the dynamics and ways of possible events, and measures of their implementation as well. This is an advantage since it enables us to realistically see the effects of oil spills on water resources and to come up with the most effective rehabilitation and response procedures to mitigate further pollution. Moreover, likewise, the results of the simulation become indispensable not only for research purposes but also for the very applications in almost environmental management and mitigating catastrophic consequences of oil spills that are made because of accidents. The data and conclusions from this research can be important for developing and implementing plans to employ safety actions at underground oil and gas can corporations and for the training and training of the personnel to cope with emergencies. Besides, ecology and sustainable development research can be based on our work which is one of the key issues relating to our environment protection goals.

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#### <sup>1\*</sup>Шалымова А.Е.,

магистр, ORCID ID: 0009-0007-3888-6686, e-mail: shalymova.aigerim@gmail.com <sup>1</sup>Исахов А.А., PhD, профессор, ORCID ID: 0000-0002-1937-8615, e-mail: alibek.issakhov@gmail.com

<sup>1</sup>Казақстан-Британ техникалық университеті, 050000, Алматы қ., Қазақстан

## АВАРИЯЛЫҚ ТӨГІЛУ КЕЗІНДЕ СУ БЕТІНЕ МҰНАЙ МЕН МҰНАЙ ӨНІМДЕРІНІҢ ТАРАЛУЫН САНДЫҚ МОДЕЛЬДЕУ

#### Андатпа

Судың ластануы бүгінгі күннің өзекті мәселесі. Мұнай өндірудің өсуіне, мұнай тасымалдаудың жаһандануына, жаңа кен орындарының қолданысқа берілуіне қарай судың мұнай өнімдерімен ластану көлемі өсіп келеді. Бұл экожүйеге зиянын тигізіп отыр. Жұмыстың мақсаты су бетіндегі мұнай өнімінің таралуын сандық модельдеу, апаттық төгілулерді оқшаулау және жою бойынша іс-шараларды жоспарлау мен жедел басқарудың тиімділігін арттыруға көмектеседі. Ластану аймағының әр жылдамдықта қалай өзгеретінін зерттеу үшін ластаушы (бензин) шығарындыларының әртүрлі деңгейлері қарастырылды. Бұл есепті модельдеу үшін математикалық модель ретінде сығылмайтын сұйықтық үшін Навье-Стокс теңдеулері қолданылды. Навье-Стокс теңдеулерінің сандық шешіміне қарапайым алгоритм арқылы қол жеткізілді. Сандық әдіс пен математикалық модельді тексеру үшін тест тапсырмасы орындалды. Есептеу нәтижелері эксперимент нәтижелерімен салыстырылып, тамаша сәйкестікті көрсетті.

Тірек сөздер: математикалық модель, мұнайдың төгілуі, судың ластануы.

## <sup>1\*</sup>Шалымова А.Е.,

# магистр, ORCID ID: 0009-0007-3888-6686, e-mail: shalymova.aigerim@gmail.com

<sup>1</sup>Исахов А.А.,

PhD, профессор, ORCID ID: 0000-0002-1937-8615, e-mail: alibek.issakhov@gmail.com

<sup>1</sup>Казахстанско-Британский технический университет, 050000, г. Алматы, Казахстан

## ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ РАСПРОСТРАНЕНИЯ НЕФТИ И НЕФТЕПРОДУКТОВ ПРИ АВАРИЙНОМ РАЗЛИВЕ НА ВОДНОЙ ПОВЕРХНОСТИ

#### Аннотация

Загрязнение воды является актуальной проблемой на сегодняшний день. Особенно растет количество загрязнений воды нефтепродуктами, так как растет добыча нефти, происходит глобализация нефтеперевозок и вводятся в эксплуатацию новые месторождения. Это пагубно влияет на экосистему. Целью работы является численное моделирование распространения нефтепродукта на водной поверхности, которое может помочь повысить эффективность планирования и оперативного управления мероприятиями по локализации и ликвидации аварийных разливов. Были рассмотрены различные скорости выбросов загрязняющего вещества (бензина), чтобы исследовать, как меняется зона загрязнения при каждой скорости. Для моделирования этой задачи в качестве математической модели использовались уравнения Навье-Стокса для несжимаемой жидкости. Численное решение уравнений Навье-Стокса было достигнуто с помощью простого алгоритма. Было выполнено тестовое задание для проверки численного метода и математической модели. Результаты расчетов были сопоставлены с результатами эксперимента и показали отличное соответствие.

Ключевые слова: математическая модель, разлив нефти, загрязнение воды.