Mathematical Model and Computer Simulation for Oil Spill in Ice Waters Around Island Based on FLUENT

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***Abstract*—The simulation of oil spill in ice waters was built by computational liquid dynamic software FLUENT. The coupling of pressure and velocity under unsteady-state conditions was solved by pressure implicit with splitting of operator algorithm. The boundary conditions of nonlinear free surface were solved by volume of fluid. And the numerical wave water flume was established by the user defined function with the help of C programming language. The whole process of the dispersion and diffusion of oil spill in ice waters was shown vividly and visually on screen in graphic mode dynamically. Also the distribution of velocity vector could be obtained. Basing on this intelligence simulation method, the movement characteristics of oil spill in ice waters were analyzed. The results showed that: with the ice sheet, the oil adhered to the ice lower surface easily, while its diffusion area was less than the one on the free sea surface in the same temperature; some oil was entrained to the ice upper surface and continued to transport, which accelerated the ice melting; the pollution area caused by oil spill near to the ice sheet was less than the one caused by oil spill far from the ice sheet. These simulation results were similar to some experimental phenomena and this computational method was validated to be effective.**

***Index Terms*—simulation, algorithm, ice waters, oil spill, software FLUENT**

I. Introduction

The recent research has shown that the northeast channel through the Canadian Arctic region is a shortcut linking Europe and Asia. In the summer of 2007, large scope of ice-free sea-surfaces first appeared. This phenomenon greatly increases the possibility of Arctic shipping route open in the future [1]. But annual temperature in the Arctic is low [2], and the ability of marine organisms to resist ship pollution is limited. Thus after the shipping route open, oil spill caused by ship collision and non-standard operation would bring much pollution and potential interference to the fragile Arctic ecosystem [3, 4]. The oil spill which has not been timely treated would contact with the Arctic organisms [5], enter the food chain gradually [6, 7], and even lead to global environment change [8]. Therefore, it is imperative to study oil spill trajectory in the Arctic environment. And computational fluid dynamics software FLUENT is a novel method.

Ice and ice-free waters have different environmental conditions: the temperature of atmosphere and seawater in arctic ice waters is lower than ice-free waters, and icy seawater temperature is close or equal to the freezing point; As ice exists as a medium in ice waters, oil spill not only interacts with atmosphere and seawater, but also is influenced by the ice, so that the behavior and consequence of oil spill becomes more complicated.

However, in the last 20 years, the computational research of forecast model on oil spill in ice waters was relatively rare. Some scholars expressed the diffusion radius of oil spill on ice in the form of formula through the small-scale experiment [9, 10]. Keevil et al. [11, 12] studied the diffusion law of oil spill under ice surface. Ross et al. [13, 14] conducted the controllable experiments to study the diffusion law of oil spill in seawaters with drifting ice. As the situations of oil spill under different circumstances were different, the oil diffusion expressions were based on the empirical formula yet. Thus the general prediction method and its wide application have not been achieved up to the present.

In this paper, we used computational fluid dynamics software FLUENT as a platform, adopted the Pressure Implicit with Splitting of Operators (PISO) algorithm to solve the coupling of pressure and velocity under unsteady-state conditions, while we used the method of Volume of Fluid (VOF) to solve the nonlinear free surface boundary problem. Also we employed the User Defined Function (UDF) of FLUENT to build numerical wave water area, with the help of C programming. Basing

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on this, the ship oil spill model was established. The whole course of oil spill drift-diffusion could be simulated dynamically. Therefore, the motion characteristics of oil spill in ice waters around island were analyzed by computer in order to propose the effective measurements for prevention and management of oil spill pollution.

II. Mathematical Model

A. Control Equation

The Euler rectangular coordinate system was used to describe the problem, where x-axis represented the horizontal direction and the right direction was positive; y-axis represented the vertical direction and the upward direction was positive.

The seawater is always in constant motion with the interaction of various forces. Therefore, the laws of mass and momentum conservation are the basic laws to dominate the seawater movement. As the fluid is incompressible and its viscosity coefficient is constant, the N-S equation is adopted as control equation for free surface flow problem.

Continuity equation and momentum equations are shown below:

$$\frac{\partial u}{\partial x}+\frac{\partial w}{\partial y}=0\,, \tag{1}$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+w\frac{\partial u}{\partial y}=-\frac{1}{\rho}\frac{\partial p}{\partial x}+\upsilon\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right], \tag{2}$$

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+w\frac{\partial w}{\partial y}=g-\frac{1}{\rho}\frac{\partial p}{\partial y}+\upsilon\left[\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}\right]. \tag{3}$$

Where u, w are velocity components in x, y direction, ρ is the fluid density, p is the fluid pressure, v is the kinematics viscosity coefficient of fluid.

Standard k-ε transport equations are shown below:

$$\begin{aligned}&\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho k u_i)}{\partial x_i}\\&=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k\end{aligned}\,, \tag{4}$$

$$\begin{aligned}&\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial(\rho\varepsilon u_i)}{\partial x_i}\\&=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right]+\\&C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k+C_{3\varepsilon}G_b\right)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon\end{aligned}\,. \tag{5}$$

Where G_k is generation item of turbulence kinetic energy k caused by the mean velocity gradient; G_b is generation item of turbulence kinetic energy k caused by the buoyancy; Y_M represents the contribution of fluctuation expansion in compressible turbulence; $G_{1\varepsilon}$, $G_{2\varepsilon}$ and $G_{3\varepsilon}$ are empirical constant; σ_k and σ_ε are the Planck constants corresponding to the turbulence kinetic energy k and the dissipation rate ε, respectively; S_k and S_ε are the user-defined source terms.

B. Volume of Fluid

Sea surface condition belongs to two-phase flow and submarine oil spill belongs to three-phase flow, which is suitable to use VOF method. This method is verified effective in some other similar simulation [15]. The volume fraction a_q is introduced as the volume of substance q in the cell. a_q=0 means null, while a_q=1 means full. q=1,2,3 represents the gas, water and oil, respectively. At nonlinear free surface, a_q should satisfy

$$\frac{\partial a_q}{\partial t}+\vec{v}\cdot\nabla a_q=0,\ \sum_{q=1}^{n}a_q=1,\ q=1,2,3...\ . \tag{6}$$

The symbol $\vec{v}$ is the average velocity of cell. As the density of each port is different through the whole flow field, we adopt (7) to calculate the density in the cell where two substances mixes together.

$$\rho=\sum_{q=1}^{n}a_q\rho_q\,. \tag{7}$$

VOF model can simulate two types of immiscible fluids by solving the separate momentum equation and processing the volume ratio of each fluid which cross the domain, expressed as below:

$$\frac{\partial}{\partial t}(\rho\vec{v})+\nabla\cdot(\rho\vec{v}\vec{v})=-\nabla P+\nabla\cdot\left[\mu\left(\nabla\vec{v}+\nabla\vec{v}^T\right)\right]+\rho\vec{g}+\vec{F}\,. \tag{8}$$

C. Linear Wave

The micro wave amplitude theory was a linear wave theory which adopted potential function to research wave motion. If wave amplitude was far less than wavelength and water depth, the nonlinear items of free surface boundary conditions could be neglected. Then the linear Airy wave was obtained. Wave surface equation and velocity potential equation was shown in (9) and (10).

$$\zeta=\frac{a}{2}\sin(kx-\omega t)\,, \tag{9}$$

$$\varphi=-\frac{ga}{\omega}\frac{ch\{k(h+z)\}}{ch(kh)}\cos(kx-\omega t)\,. \tag{10}$$

Where a was wave height; z was water depth; ω was circular frequency which represented the number of vibration in the time range of 2π; k was the wave number. The relationships of circular frequency (ω), wavelength (λ), wave velocity (c) and cycle (T) were shown in (11) to (13).

$$\omega^2=gk\cdot\frac{e^{kh}-e^{-kh}}{e^{kh}+e^{-kh}}\,, \tag{11}$$

$$\lambda = \frac{gT^2}{2\pi} th(kh) = \frac{gT^2}{2\pi} th(\frac{2\pi}{\lambda} h) , \tag{12}$$

$$c = \frac{\lambda}{T} = \frac{gT}{2\pi} th(\frac{2\pi}{\lambda} h) . \tag{13}$$

According to the relationship of velocity potential and velocity, the motion velocity of any seawater particle could be obtained in (14) and (15). According to (11) - (13), the motion trajectory of seawater particle was obtained in (16) and simplified in (17).

$$u = \frac{gka}{\omega} \cdot \frac{ch[k(h+z)]}{ch(kh)} \cdot \sin(kx - \omega t) , \tag{14}$$

$$w = -\frac{gka}{\omega} \cdot \frac{sh[k(h+z)]}{ch(kh)} \cdot \cos(kx - \omega t) , \tag{15}$$

$$\frac{(x-x_0)^2}{\left\{ a\dfrac{ch[k(h+z_0)]}{sh(kh)} \right\}^2} + \frac{(z-z_0)^2}{\left\{ a\dfrac{sh[k(h+z_0)]}{sh(kh)} \right\}^2} = 1 , \tag{16}$$

$$(x-x_0)^2 + (z-z_0)^2 = (ae^{kz_0})^2 . \tag{17}$$

Eq. (16) represented that the motion trajectory of seawater particle for linear wave was a circle. Furthermore, its radius decreased rapidly while water depth ($-z_0$) increasing. When it came to a certain depth, the motion disappeared. This properties were considered in C program of UDF.

III. Computer Simulation

Some assumptions were made for the model: the impact of ship shaking on the oil level in tank was not considered; the three-phase flow of oil, water and gas was not compressible and not inter-miscible; the oil spill process was adiabatic and the three phases were isothermal flow, regardless of thermal exchange among different phases; there was no broken ice in the seawaters.

One side of ship was cracked by some external force and the cleft was in the opposite direction of ocean current. The oil tank was rectangular and it contained the diesel of 985*kg/m*^{3}. The upper part of calculation area was atmosphere, while the lower part was water with ice sheet covered on the right surface, as shown in Fig. 1. The grids of the whole calculation domain were rectangular.

The two-dimension, unsteady and separated implicit solver was adopted. The number of phases in VOF model was set to 3, where air was the basic phase, water was the second phase and oil was the third phase. The Geo-Reconstruct was used as the free surface reconstruction format. The reference pressure was set to be the standard atmospheric pressure and the value of working fluid density was set to be 1.225*kg/m*^{3} in the operation environment, while the gravity was considered.

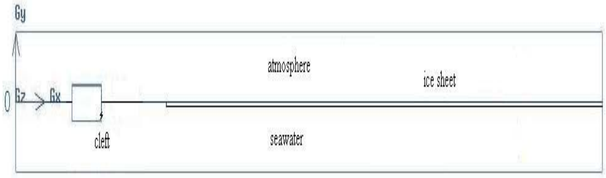

Figure1. Schematic diagram of numerical water area

The velocity inlet was on the left of the model, while the velocity outlet was on the right. At initial time, the calculation domain was initialized, and the water volume fractions above and below the free surface were set to 0 and 1, respectively. The direction of current velocity was set perpendicular to the left inlet boundary. The top boundary was set to pressure inlet, whose direction was perpendicular. The bottom of the domain was set to wall. The cleft of oil tank was set to the boundary condition of interior, and the other parts were set to the boundary condition of wall. PISO algorithm based on pressure solution was adopted to solve the coupling problem of pressure and velocity under unsteady states, and was used by some researchers for fire and explosion prediction [16]. The time step of numerical calculation was 0.005s. The flow chart for FLUENT simulation is shown in Fig. 2.

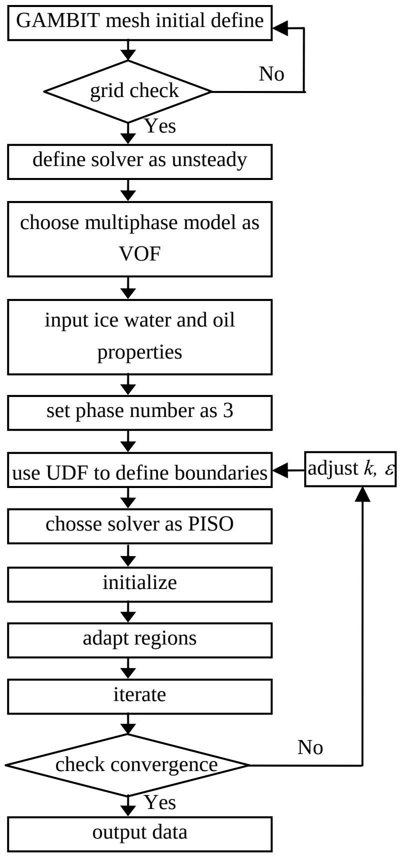

Figure 2. Flow chart for software simulation

The wave was one of important ocean motion forms and could appear from ocean surface to interior. In order to simulate damaged ship oil spill in Arctic shipping route more precisely, the oil motion in ice water with the interaction of wave and current was simulated, taking linear simple harmonic wave for example. The properties of oil and seawater were given below: the oil kinematics viscosity coefficient and surface tension coefficient were υ_0=1.053×10^{-5}m^2/s and σ_0=200$\mu N/cm$, respectively. The seawater density was ρ_w=1025kg/m^2, and kinematics viscosity coefficient was υ_w=1.7×10^{-6}m^2/s.

As artificial viscosity method was insensitive to the frequency or wavelength of incoming wave, and was more effective to adsorb incoming waves with different frequency or wavelength, this method was a good wave adsorbing method for establishing a general numerical wave flume. Therefore, the artificial viscosity method was adopted in order to prevent the interference of wave reflection in flume. The essential of this method was to add damping term in the wave adsorption section. In addition, the length of wave adsorption section should be one time of incoming wavelength, as the effects on wave adsorption was related to the length of wave adsorption section.

The interaction process of ocean wave and current can be separated to three stages. The wave and current exist independently at the first stage, mix at the second stage and form steady union at the third stage. Therefore, the value of velocity was superimposed by the velocities of wave and current:

$$u = u_0 + \frac{gka}{\omega} \cdot \frac{ch[k(h+z)]}{ch(kh)} \sin(kx - \omega t)\,. \qquad (18)$$

The symbol of u_0 represented the seawater current velocity. When wave and current coexisted, the energy conservation of them should be considered for wave adsorption. In order to achieve energy conservation, outflow boundary conditions were set corresponding to inflow boundary conditions besides wave adsorption section.

The flume model with wave source is illustrated in Fig. 3. The wave point source of vertical distribution is set on the left of flume, while damping wave adsorption section is set on the right. The potential flow theory is suitable for the whole flow field. The damping coefficient of μ is zero on the surface facing waves in wave adsorption section, which make potential function continuous variation. Then μ is the linear function of x. S_1 stands for the right and left boundaries. W stands for the bottom boundary of flume. The up free surface is pressure boundary. S_1 and S_2 are computational domains, among which S1 is damping wave adsorption.

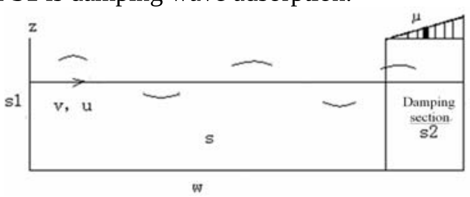

Figure 3. Wave flume model

The source term, the initial conditions and boundary conditions are defined by the macro of DEFINE_SOURCE (my_source_x, c, t, dS, eqn), DEFINE_INIT (my_init_function, domain), DEFINE _PROFILE (x_velocity_in, thread, index), DEFINE _PROFILE (y_velocity_in, thread, index) and DEFINE _PROFILE (voffactor, thread, index), respectively， which was shown in Appendix A. The result of simulation is shown in Fig. 4.


Figure 4. Wave profile

IV. Simulation Validation

The trajectory of the oil spilled from the oil tank was shown in Fig. 5 to Fig. 9, where the yellow, light blue and dark blue areas stood for the air, water and oil, respectively. In each figure, picture (a) stood for the condition of oil spill site closer to the ice sheet, while picture (b) was for the far site and picture (c) was for the condition of oil spill site closer to the ice sheet with nulclear wave.

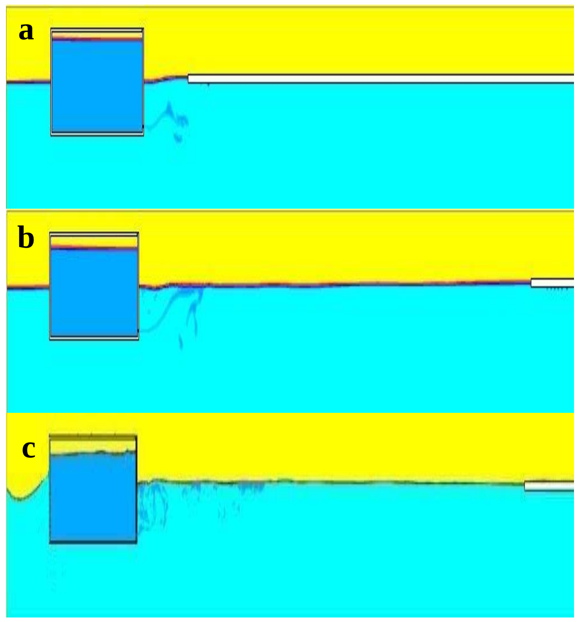

Figure 5. Distribution of oil-water-air at time of 10s

For the different liquid levels in and out of oil tank at initial time, the oil injected through the cleft and formed jet or plume into the external seawater, and was quickly broken up to the droplets by the coming flow. As the density of oil was less than that of water, the oil floated upwards in the form of droplets group by the water buoyancy. At the mean time, the oil group inclined to the spreading direction of ocean currents with the carrying action of coming flow. When the oil spill site was close to the ice sheet, the rising oil droplets would be intercepted by the edge of ice and adhere to the lower surface of ice, after the oil reached the ice sheet as shown in Figure 5a. When the oil spill site was far from the ice sheet, the oil would not reach the ice sheet within a short time and could easily rise to the sea surface without any barrier, as shown in Fig. 5b. The obvious water particles circle motion appeared to the inverse direction of wave transmission. Contrary to this phenomenon, the violent extent of motion decreased along the direction of wave transmission near surface, as shown in Fig. 5c. The wave promoted the dispertion and transport of the oil.

With the fluid level in oil tank falling gradually over time, the pressure difference inside and outside changed lower and lower. This led to the amount and velocity of oil spill declining gradually. Thus the concentration of oil near the tank cleft decreased significantly. At this time, the oil floated gradually along the wake flow trajectory of previous oil droplets, with the action of sea current and water buoyancy. When the oil spill reached sea surface, oil became to expand in the form of oil film with the action of gravity and surface tension. And the thickness of oil film became less, along with the oil expanding scope increasing.

At the condition of oil spill site near to the ice sheet, the spreading and diffusion of oil film was influenced by the lower surface of ice. The diffusion velocity was lower because of the friction force action. Thus the diffusion distance of oil film was significantly less than that on the free sea surface at the same temperature. This phenomenon was shown in Fig. 6.

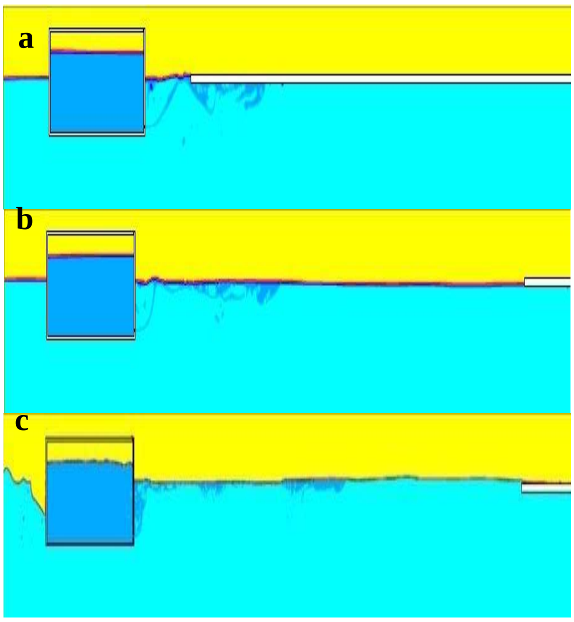

Figure 6. Distribution of oil-water-air at time of 20s

In addition, the spreading oil film could be blocked by ice and easily formed the vortex at the edge of ice sheet. Then some oil would be entrained to the ice sheet surface and continued to spread and diffuse by the action of subsequent flow, as shown in Fig. 7. And Fig. 7 was for the velocity vector distribution under the conditions of oil spill site closer to the ice sheet. This simulation result was very similar to the early phenomenon of the oil field experiment made in the Canadian arctic high latitudes by Comfort et al. [17]. That is: when the oil spill site was close to the ice sheet, some oil would transport onto the ice surface and would be absorbed by the snow or carried away by wind over time; As a result, the oil on the ice surface reduced or even disappeared finally; This phenomenon would have a significant impact on the Arctic environment; The presence of oil would increase the probability of ice melting and shorten the melting time of ice sheets; The sunlight absorption by ice sheet with oil was 30% higher than the regular ice sheet, and the melting time would be advanced by about 7 to 21 days.

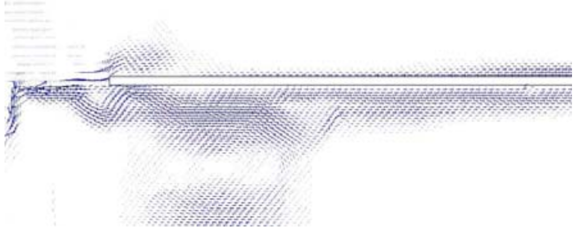
Fig.7. Velocity vector near the ice sheet edge at 20s

With time passing by, some oil could be scoured by seawater to form various sizes of droplets and dispersed in different depths of water. The large size droplets floated gradually and reaggregated with oil film on the sea surface, while the small size ones suspended in water for a long period of time. As the temperature of Arctic areas was lower than others, the viscous resistance between oil and water was relatively high, which led to the lower velocity of oil spills spreading and moving. Moreover, since the water temperature was low and even close to zero, the discretization of oil spill was not obvious in ice waters, while this action occurred obviously in a fully open free surface of no ice waters. Thus the thick oil film was easy to form on the icy sea surface, as shown in Fig. 8.

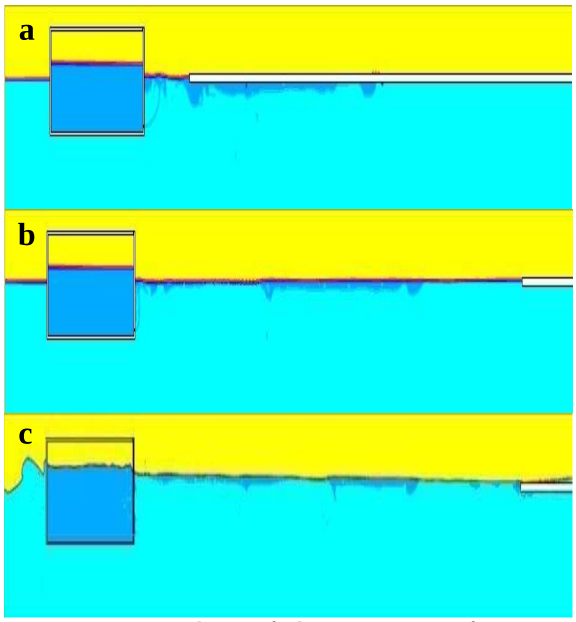

Figure 8. Distribution of oil-water-air at time of 40s

In addition, besides the characteristics mentioned above, there were other obvious differences between the oil film close to and far from the ice sheet. As shown in Fig. 8a, the oil film which was generated from the oil spill site close to the ice would float beneath the ice sheet. And for the friction action of the lower ice surface, the transport velocity of oil film was lower than that on free water surface. Therefore, its oil film area was less than the one generated from the oil spill site far from the ice sheet.

As illustrated in Fig. 9a, the oil droplets below water would float to the lower ice surface and gathered gradually for barrier of ice sheet. This computational simulation was the same to the experiment results, which was obtained by Greene [18]. In his laboratory experiment, the icy water tank was applied to research the movement of oil spill beneath the ice sheet surface, and the phenomenon of a certain thickness oil film forming under the ice sheet was observed. At this time, because the pressure difference between internal and external of oil tank decreased to 0, the oil in tank would not spill any more, while the spilled oil transported and diffused gradually in the form of oil film with the action of sea water current.

At the condition of oil spill site far from ice sheet, as shown in Fig. 9b, the oil was blocked by the edge of ice sheet after it reached sea surface. This simulation was similar to the phenomenon shown in Fig. 6a: some oil was entrained to the ice surface by the action of vortex and would disappear over time for weathering. On the other hand, most of oil would transport toward the lower ice sheet surface and diffused downstream with sea water. Because this part of oil would not contact with air and there was no weathering action here, it required people to adopt remedial measures to clean up. It could be drawn from Fig. 6b that oil amount spilling out of the tank was more than that in Fig. 6a. Thus the oil film in Fig. 6b was far thicker than that in Fig. 6a and it was easier to recover.

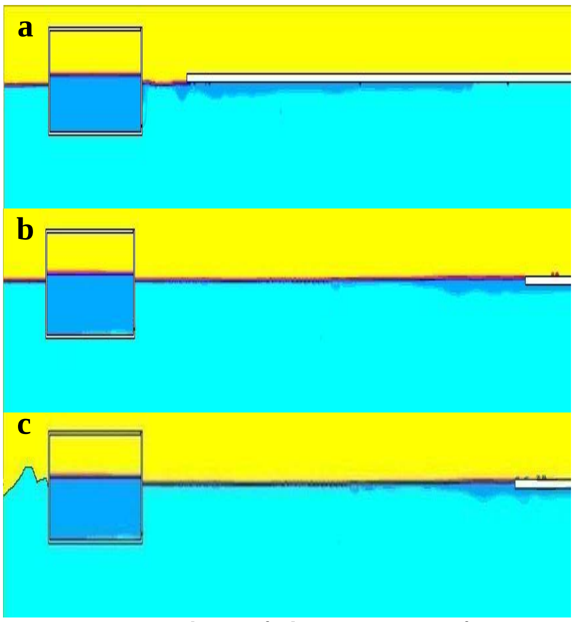

Figure 9. Distribution of oil-water-air at time of 100s

In this mathematics and computational simulation process, the residuals of x velocity, y velocity and continuity were monitored simultaneously and shown in Fig. 10. The residuals of y velocity less than 1×10^{-5}, the residuals of x velocity less than 1×10^{-3} and the residuals of continuity less than 1×10^{-3} indicated that this mathematics simulation method could simulate the oil spill in icy waters with less errors.

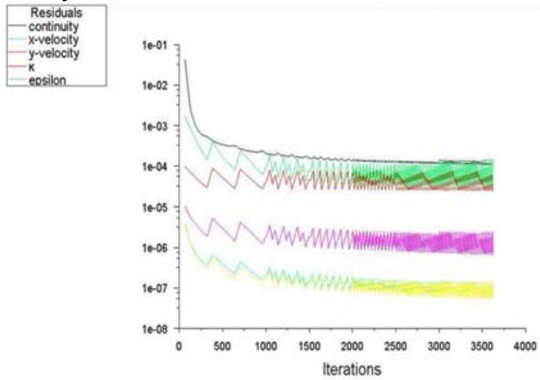

Figure 10. Residuals of continuity, x, y velocity, k and ε

V. Conclusions

In this paper, we proposed a computational method to simulate the trajectory of oil spill in icewaters around island. The computational liquid dynamic software FLUENT was adopted. The numerical water flume was established by UDF of FLUENT with the help of C program language. The PISO algorithm was used to solve the coupling of pressure and velocity under unsteady-state conditions, while the method of VOF was used to solve the nonlinear free surface boundary problem. On this basis, the model of oil spill influenced by sea current , ice and wave was researched. The results showed that the simulation of oil spill was similar to some previous laboratory experiments phenomena, which indicated that our proposed computational technique based on software FLUENT was an effective method for oil spill simulation in ice waters.

Appendix A Program Implementation of Macro

```
DEFINE_PROFILE(x_velocity_in,thread,index)
{
  real x[ND_ND];
  real y;
  face_t f;
  real  t;
  real  u;
  t=RP_Get_Real("flow-time");
  begin_f_loop(f,thread)
    {
      F_CENTROID(x,f,thread);
      y = x[1];
      if(y<(a*cos(w*t)))
           u=a*w*cosh(k*(y+h))*cos(-w*t)/sinh(k*h)+ux;
          /*                    u=a*w*cosh(k*(y+h))*cos(-
w*t)/sinh(k*h)+ux;*/
      else u =0.0;
           F_PROFILE(f,thread,index)=u;
    }
  end_f_loop(f,thread)
}

DEFINE_PROFILE(voffactor,thread,index)
{
```

```
    real x[ND_ND];
    real y;
    face_t f;
    real  t;
    t=RP_Get_Real("flow-time");
    begin_f_loop(f,thread)
      {
       F_CENTROID(x,f,thread);
       y = x[1];
       if(y<(a*cos(w*t)))
       F_PROFILE(f,thread,index) = 1.0;
       else F_PROFILE(f,thread,index) = 0.0;
      }
    end_f_loop(f,thread)
  }

  DEFINE_SOURCE(my_source_x,c,t,dS,eqn)
  {
          real x[ND_ND];
          real mu,source;
          C_CENTROID(x,c,t);
          mu=10*x[0];
          source=-mu*C_U(c,t);
          dS[eqn]=-mu;
          return source;
  }

  DEFINE_INIT(my_init_function, domain)
  {
          cell_t c;
          Thread *t;
          real x[ND_ND];
          thread_loop_c (t,domain)
          {
                  begin_c_loop_all (c,t)
                  {
                          C_CENTROID(x,c,t);
                          /*        if (x[1]<0)*/
                          C_U(c,t)=0.0;
                          C_V(c,t)=0.0;
                  }
                  end_c_loop_all (c,t)
          }
  }
```

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