

Izviren kombiniran večfazni model mešalne faze eksplozije pare

An Original Combined Multiphase Model of the Steam-Explosion Premixing Phase

Matjaž Leskovar - Borut Mavko

V večfaznem toku so lahko faze razporejene tako, da večfaznega toka ni mogoče obravnavati niti samo z modeli proste površine niti samo z modeli večfaznega toka. Takšno porazdelitev faz srečujemo na primer pri izotermnih preskusih mešalne faze eksplozije pare, kjer razpršene kroglice prodirajo v vodo, medfazna ploskev voda - zrak pa se ne razprši in ostane ostra. Pri modeliranju izotermnih mešalnih preskusov so običajno obravnavane vse tri faze, to so voda, zrak in kroglice, enakovredno z modeli večfaznega toka. Tako je obravnavana medfazna ploskev voda - zrak kot razpršen tok mehurčkov zraka v vodi oziroma kapljic vode v zraku, kar je fizikalno neustrezna slika in zaradi togih medfaznih sklopitvenih členov tudi numerično težko rešljiva naloga. Zato smo si zamislili, da bi izotermni mešalni proces obravnavali z izvirnim kombiniranim večfaznim modelom, pri katerem bi kroglice obravnavali kot običajno z modelom večfaznega toka, medtem ko bi medfazno ploskev voda - zrak obravnavali z modelom proste površine.

Z razvitim kombiniranim večfaznim modelom smo simulirali izotermni preskus Q08, ki so ga izvedli na napravi QUEOS. Najbolj problematičen del simuliranja izotermnega mešalnega preskusa je pravilna napoved plinskega stebra, ki se oblikuje med prodiranjem kroglic v vodo. Da bi bolje spoznali, kako se plinski steber oblikuje, smo opravili obsežno parametrično analizo (velikost mreže, začetno debelino medfazne ploskve voda - zrak, gostoto vode, položaj vključitve medfazne sklopitve gibalne količine). Ugotovili smo, da se plinski steber oblikuje tako kakor pri preskusu le, če v modelu medfazno trenje kroglic na vodni gladini obravnavamo na poseben način, ki upošteva nezveznost prehoda zrak - voda.

© 2002 Strojniški vestnik. Vse pravice pridržane.

(Ključne besede: tok večfazni, modeli večfazni, eksplozija parne, metode z nivojsko funkcijo, simuliranje)

In multiphase flow, different phase distributions can occur that cannot be adequately modeled with just free-surface models or with just multiphase models. Such a distribution of phases occurs, for example, in isothermal steam-explosion premixing experiments, where dispersed spheres penetrate the water and the water-air surface remains sharp. A common practice when modeling isothermal premixing experiments is to treat all three phases involved – the water, the air and the spheres' phase – equally, with multiphase flow models. In this way the water-air surface is treated as a dispersed flow of bubbles in water or droplets in air, which is a physically incorrect picture and because of very strong momentum-coupling terms also numerically not an easily solvable problem. Therefore, we decided to develop an original, combined multiphase model, where the spheres are treated, as is usual, with a multiphase flow model, whereas the water-air surface is treated with a free-surface model.

The QUEOS isothermal premixing experiment Q08 was simulated with the developed combined multiphase model. A crucial part in isothermal premixing experiment simulations is the correct prediction of the gas chimney, which forms during the spheres' penetration into the water. To get a better understanding of the gas-chimney formation an extensive parametric analysis (mesh size, initial water-air surface thickness, water density, interfacial momentum-coupling starting position) was performed. We established that the right gas-chimney formation can be obtained if a special spheres' drag treatment at the water-air surface, which considers the discontinuous air-water transition, is incorporated into the model.

© 2002 Journal of Mechanical Engineering. All rights reserved.

(Keywords: multiphase flow, multiphase models, steam explosion, level set methods, simulations)

0 UVOD

Porazdelitev faz v večfaznem toku je lahko različna. Tako so lahko faze na primer razporejene v večja območja, ki so med seboj ločena z gladko medfazno

0 INTRODUCTION

In multiphase flow different phase distributions can occur, these range from unmixed-phase distributions, where the phases are arranged

ploskvijo (npr. stratificiran tok). Takšne večfazne tokove opisujemo z modeli proste površine, ki temeljijo na reševanju Navier-Stokesovih enačb ob upoštevanju medfaznih robnih pogojev. Drugo skrajnost pomenijo večfazni tokovi z razpršenimi fazami (npr. mehurčkast tok), pri katerih je medfazno ploskev praktično nemogoče spremljati in jih zato opisujemo z modeli večfaznega toka, ki temeljijo na manj natančnih povprečenih Navier-Stokesovih enačbah. Med tema obema skrajnostma (ločene faze – razpršene faze) obstajajo še številne porazdelitve faz, ki jih ni mogoče obravnavati niti samo z modeli proste površine niti samo z modeli večfaznega toka. Te porazdelitve faz lahko razdelimo v dve skupini. Prvo skupino predstavljajo tiste porazdelitve faz, pri katerih so faze razpršene le na določenih območjih, medtem ko so druge ločene z gladko medfazno ploskvijo [1]. Takšna porazdelitev faz se pojavi na primer v kasnejši fazi razvoja Kelvin-Helmholtzove nestabilnosti. Drugo skupino pa predstavljajo tiste porazdelitve faz, pri katerih so nekatere faze ločene z gladko medfazno ploskvijo, medtem ko so druge faze razpršene. Takšno porazdelitev faz srečamo na primer pri izotermnih preskusih mešalne faze eksplozije pare, pri katerih spuščajo različne curke hladnih kroglic v posodo, napolnjeno z vodo [2].

V tem prispevku bomo predstavili izvirni kombinirani večfazni model, ki smo ga razvili za modeliranje izotermnih preskusov mešalne faze parne eksplozije [3]. Nova zasnova obravnave večfaznih tokov je dovolj splošna, da jo je mogoče preprosto prilagoditi tudi za obravnavo vseh drugih porazdelitev faz druge obsežne skupine faznih porazdelitev.

1 MODELIRANJE VEČFAZNEGA TOKA

Pri modeliranju izotermnih mešalnih preskusov so običajno obravnavane vse faze, to so voda, zrak in kroglice, enakovredno z modeli večfaznega toka [4]. Ti modeli večfaznega toka temeljijo na predpostavki, da vsaka faza z določeno fazno verjetnostjo kot oblak zaseda celotno simulirno območje in da so faze med seboj povezane z medfaznimi sklopitvenimi členi.

Značilnost izotermnih mešalnih preskusov je, da ostaneta voda in zrak med celotnim preskusom ločena z gladko medfazno ploskvijo, kakor je shematično prikazano na sliki 1, kjer so predstavljene tri mrežne celice. Indeks a in w označujeta fazi zraka in vode, $\Delta \vec{v}_{aw}$ pa je razlika vektorjev hitrosti zraka in vode. Pri modelu večfaznega toka opisujemo medfazno ploskev voda - zrak kot razpršen tok mehurčkov zraka v vodi oz. kapljic vode v zraku (sl. 1), kar je fizikalno neustrezna slika. Ker so medfazni sklopitveni členi gibalne količine v razpršenih tokovih, pri katerih je razmerje gostot faz veliko, togi, so pri izrecnih numeričnih metodah potrebni zelo majhni časovni koraki, pojavijo pa se tudi težave s konvergenco [5]. Poleg tega se medfazna ploskev voda - zrak numerično razprši zaradi numerične difuzije

in larger regions separated by a smooth interface (for example, stratified flow), to mixed distributions, where the phases are dispersed and it is practically impossible to track the phase interfaces (for example, bubbly flow). In between there is a variety of phases' distributions, which cannot be adequately modeled with just free-surface models, which are based on Navier-Stokes equations that consider the interface boundary conditions, or just with multiphase flow models, which are based on less accurate, averaged Navier-Stokes equations. In general, these phase distributions can be classified in two groups. The first group comprises cases where the phases are only dispersed in some domains, whereas elsewhere the phase interfaces are smooth [1]. Such a phase distribution occurs, for example, at a late stage of the Kelvin-Helmholtz instability. The second group comprises cases where some phases are separated with a smooth interface, whereas the other phases are dispersed. Such a phase distribution occurs, for example, in isothermal steam-explosion premixing experiments, where different jets of cold spheres are injected into a water pool [2].

In this paper an original combined multiphase model developed for isothermal steam-explosion premixing experiments modeling will be presented [3]. This new concept of multiphase-flow treatment is general enough for it to be easily adapted to all other cases of phase distribution of the comprehensive second-phase distributions group.

1 MULTIPHASE FLOW MODELING

A common practice in isothermal premixing experiments modeling is to treat all three phases involved – the water, the air and the spheres' phase – equally with multiphase flow models [4]. These multiphase flow models are based on the assumption that each of the phases occupies, with a given phase-presence probability, the whole simulated region as a cloud, and that the phases interact through interfacial coupling terms.

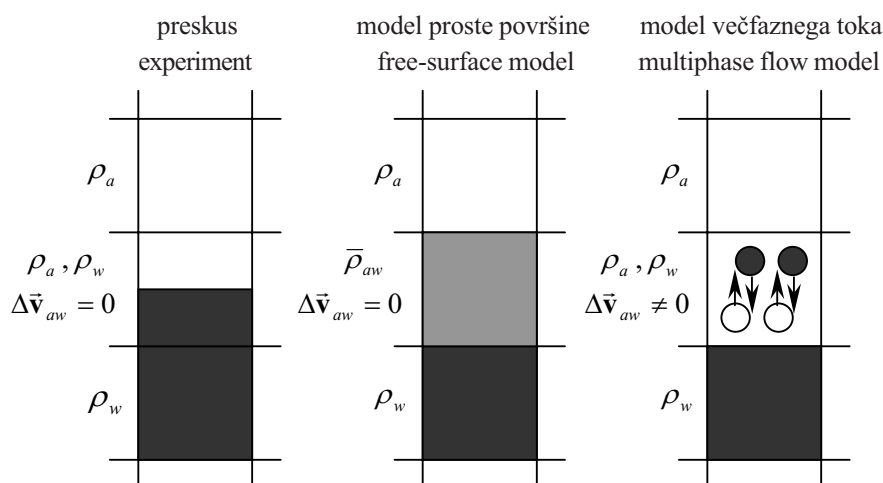
The special feature of isothermal premixing experiments is that the water and air phases remain separated by a free surface during the whole experiment, as shown schematically in Figure 1, where three mesh cells are presented. The indices a and w correspond to the air and water phases and $\Delta \vec{v}_{aw}$ is the difference between the air- and water-velocity vectors. In the multiphase flow model the water-air surface is treated as a dispersed flow of air bubbles in water or water droplets in air (Fig. 1), which is a physically incorrect picture. Since the interfacial momentum coupling terms in dispersed flows of fluids with high density ratios are very stiff, convergence problems occur and in explicit numerical methods extremely small time steps have to be used [5]. In addition, since in multiphase flow models

[6], ker pri modelih večfaznega toka medfazni ploskvi ne posvečamo posebne pozornosti. Zato smo se odločili, da bomo medfazno ploskev voda - zrak obravnavali z modelom proste površine in tako odpravili vse omenjene pomanjkljivosti obravnave medfazne ploskve z modelom večfaznega toka, ki ni primeren za takšne probleme.

Pri modelih proste površine uporabljamo za zasledovanje stične površine posebne algoritme, na stični površini pa vzamemo povprečne lastnosti faz (sl. 1). Ker se faze ne mešajo, zadošča za opis večfaznega toka eno hitrostno polje. Formalno lahko zato vodo in zrak obravnavamo kot eno, združeno fazo z nezveznimi faznimi lastnostmi na medfazni ploskvi voda - zrak in tako lahko izotermni mešalni potek obravnavamo kot navidez dvofazen tok razpršenih kroglic v kontinuumu združene faze voda - zrak. To je bistvo izvirnega kombiniranega večfaznega modela, pri katerem kroglice obravnavamo z modelom večfaznega toka, združeno fazo voda - zrak pa z modelom proste površine.

no special attention is given to the phases' interface, the water-air surface numerically spreads due to numerical diffusion [6]. Therefore, we decided to treat the water-air surface with a free-surface model and suppress, in this way, all the mentioned drawbacks of treating the phases' interface with multiphase flow models, which are not suited for such problems.

In free-surface models special interface-tracking algorithms are used, and since the phases do not mix the phases' flow is described with only one velocity field. At the phase interfaces the average phase properties are taken (Fig. 1). In this way the water and air phases can be regarded as a single, joint phase with discontinuous phase properties at the water-air interface, and consequently the isothermal premixing process can be treated as a quasi two-phase flow of dispersed spheres in the continuous joint water-air phase. This is the essence of the original combined multiphase model, where the spheres are treated with a multiphase flow model and the joint water-air phase with a free-surface model.



Sl. 1. Obravnava medfazne ploskve voda - zrak pri modelu proste površine in modelu večfaznega toka
Fig. 1. Water-air surface treatment in the free-surface model and the multiphase flow model

2 METODA Z NIVOJSKO FUNKCIJO

Vsako fazo v tako definiranim navidez dvofaznem toku, razpršeno fazo kroglic in kontinuum združene faze voda - zrak, smo opisali s kontinuitetno in gibalno enačbo, kar je opisano v [7] in [8]. Medfazno ploskev voda - zrak smo določevali z metodo z nivojsko funkcijo [9], ki je namenjena reševanju problemov s stično površino in se v zadnjih letih veliko uporablja. Pri metodi z nivojsko funkcijo modeliramo medfazno ploskev kot ničelno izohipso $\phi = 0$ gladke nivojske funkcije, ki je definirana na celotnem obravnavanem območju kot $\phi(\vec{r}, t) = \pm d(\vec{r})$, kjer je $d(\vec{r})$ najmanjša razdalja do medfazne ploskve pri začetnem času $t = 0$. Glavne lastnosti nivojske funkcije so, da je v področju ene faze pozitivna, v področju druge faze negativna in da je gladka. Časovni razvoj lege medfazne ploskve določujemo z enačbo nivojske funkcije:

2 THE LEVEL-SET METHOD

Each phase in the so-defined quasi two-phase flow – the dispersed spheres' phase and the continuum joint water-air phase – was described using the continuity and momentum equations as explained in [7] and [8]. The water-air surface was determined using the front-capturing level-set method [9], which was developed for free-surface problems and has been widely used in recent years. In the level-set method the phases' interface is modeled as the zero set $\phi = 0$ of a smooth signed normal distance function, defined on the entire physical domain as $\phi(\vec{r}, t) = \pm d(\vec{r})$, where $d(\vec{r})$ is the signed minimum distance from the two-fluid interface at the initial time $t = 0$. The interface position is determined by solving the Hamilton-Jacobi-type level-set equation on the whole domain:

$$\frac{\partial \phi}{\partial t} + (\vec{v} \cdot \nabla) \phi = 0 \quad (1),$$

ki pomika ničelno izohipso nivojske funkcije tako, kakor se premika stična površina. Ker je ϕ gladka funkcija, v nasprotju z gostoto združene faze voda - zrak, ki je na medfazni ploskvi nezvezna, numerično reševanje enačbe nivojske funkcije (1) ni problematično. Gostota združene faze voda - zrak je določena z nivojsko funkcijo kot:

$$\rho(\phi) = \begin{cases} \rho_w, & \phi > 0 \\ (\rho_w + \rho_a)/2, & \phi = 0 \\ \rho_a, & \phi < 0 \end{cases} \quad (2).$$

Če bi predpis (2) uporabljali dosledno, bi dobili stopničast, nezvezen potek gostote in pojavile bi se nestabilnosti, ki bi bile še posebej izrazite pri velikih razmerjih gostot. Zato je priporočljivo potek gostote na medfazni ploskvi nekoliko zgladiti z:

$$\rho(\phi) = \begin{cases} \rho_w, & \phi > \varepsilon \\ \frac{(\rho_w + \rho_a)}{2} + \frac{(\rho_w - \rho_a)}{2} \left(\frac{\phi}{\varepsilon} + \frac{1}{\pi} \sin\left(\frac{\pi\phi}{\varepsilon}\right) \right), & |\phi| \leq \varepsilon \\ \rho_a, & \phi < -\varepsilon \end{cases} \quad (3),$$

kjer je ε izbrana debelina medfazne ploskve. Pri naših izračunih smo za debelino medfazne ploskve vzeli priporočeno vrednost $\varepsilon = \frac{3}{2} \Delta h$, kjer je Δh mrežna razdalja.

Na začetku izračuna je vrednost ϕ enaka pozitivni oz. negativni najmanjši razdalji do medfazne ploskve, kasneje pa to ne drži več, saj enačba (1) nivojsko funkcijo spremeni. Da bi ohranili nespremenljivo debelino medfazne ploskve, moramo ϕ po vsakem časovnem koraku ponovno določiti tako, da zopet pomeni oddaljenost od medfazne ploskve. To izvedemo s tem, da poiščemo ustaljeno rešitev enačbe:

$$\frac{\partial \phi}{\partial t} = \text{sign}(\phi_0) (1 - |\nabla \phi|), \quad \phi(\vec{r}, 0) = \phi_0(\vec{r}) \quad (4),$$

kjer je ϕ_0 izračunana nivojska funkcija po času t . Rešitev enačbe (4) ima enak predznak in enako ničelno izohipso kakor ϕ_0 in ker rešitev izpolnjuje pogoj $|\nabla \phi| = 1$, je vrednost ϕ enaka pozitivni oz. negativni najmanjši razdalji do medfazne ploskve.

3 PARAMETRIČNA ANALIZA

S kombiniranim večfaznim modelom smo simulirali preskus Q08 [10], kakor je opisano v [8], vendar brez posebne obravnave medfaznega trenja kroglic na vodni gladini. Na sliki 2 so predstavljeni rezultati simuliranja. Slika prikazuje gostoto združene faze voda - zrak (črni obrisi), fazno verjetnost kroglic (sivi obrisi) in hitrostno polje združene faze voda - zrak v valjnem koordinatnem sistemu (r, z) v ekvidistančnih 25 ms dolgih časovnih razmikih. Kakor je razvidno na sliki, se začne plinski steber, ki nastane med prodiranjem kroglic v vodo, zapirati na vrhu stebra, kar ni v skladu z opažanji pri preskusih. Na

which moves the zero level of ϕ in exactly the same way as the actual two-fluid interface moves. Since ϕ is a smooth function, unlike the density of the joint water-air phase, which undergoes a jump at the water-air interface, the level-set equation (1) is more easily solved numerically. The density of the joint water-air phase is determined from the level-set function as:

If this prescription (2) were to be used in a straightforward way a graded solution would result and instabilities would occur, especially for large density ratios. Therefore, it is recommendable to smooth the density at the interface as:

where ε is the chosen interface thickness. In our computations the recommended value $\varepsilon = \frac{3}{2} \Delta h$ was used, where Δh is the grid spacing.

It should be noted that while ϕ is initially a distance function it will not remain so at later times since the level-set equation (1) deforms it. To keep the interface thickness fixed in time the level-set function has to be reinitialized at each time step so that it remains a distance function. The reinitialisation is carried out by solving the equation:

for the steady-state solution, where ϕ_0 is the calculated level-set function at time t . The solution of equation (4) will have the same sign and the same zero level-set as ϕ_0 , and since it satisfies $|\nabla \phi| = 1$, it will be a distance function.

3 PARAMETRIC ANALYSIS

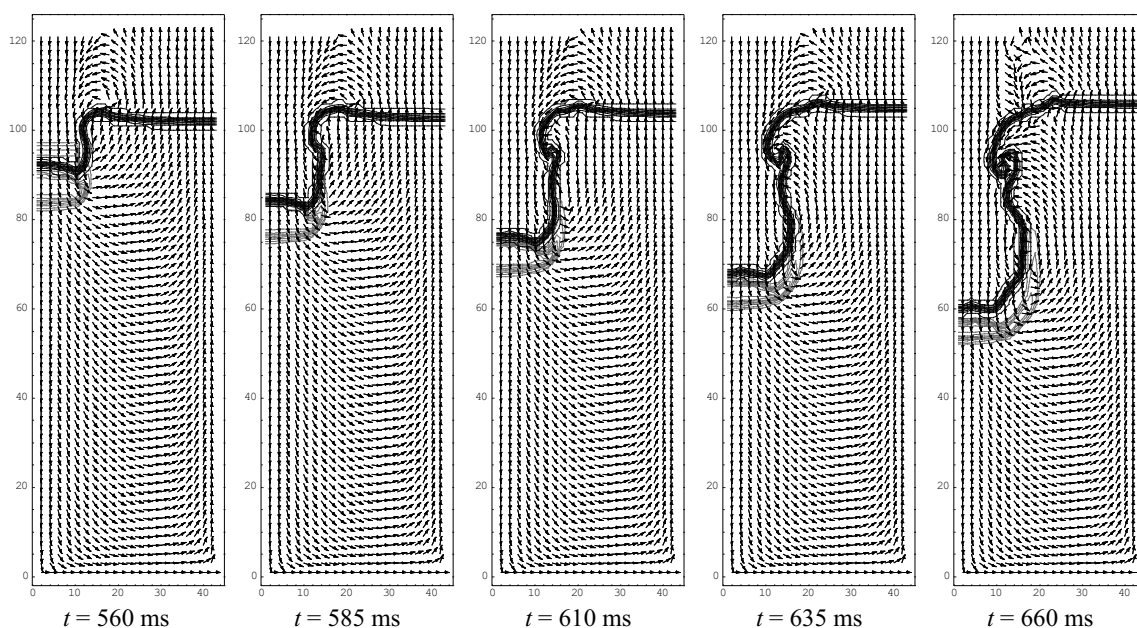
With the combined multiphase model the premixing experiment Q08 [10] was simulated, as described in [8], but without the special spheres' drag treatment at the water-air surface. The results of the simulation are presented in Figure 2. The figure shows the joint water-air phase density (black contours), the spheres' presence probability (gray contours) and the joint water-air phase velocity field in the cylindrical coordinate system (r, z) in equi-distant 25-ms-long time intervals. As seen in the figure, the gas chimney, which forms during the spheres' penetration into the water, starts to close at the top of the chimney, which is not in accordance with the experimental

sliki 3 so prikazani posnetki vseh opravljenih izotermnih mešalnih preskusov QUEOS. Poleg preskusa Q08, ki smo ga simulirali, so predstavljeni še preskusi Q01, Q02, Q05 in Q06, ki se med seboj razlikujejo po premeru kroglic, snovi, iz katere so kroglice, in skupni masi kroglic [11]. Na vseh posnetkih je jasno vidno, da se plinski steber prične zapirati na sredini in ne na vrhu, tako kakor pri simuliranju.

Da bi ugotovili, zakaj so rezultati simuliranj kakovostno napačni, smo opravili obsežno parametrično analizo. Ker geometrijska oblika modela preskusa Q08, predstavljenega v [8], ni primerna za preprosto parametrično analizo vpliva velikosti mreže, smo parametrično analizo opravili v nekoliko

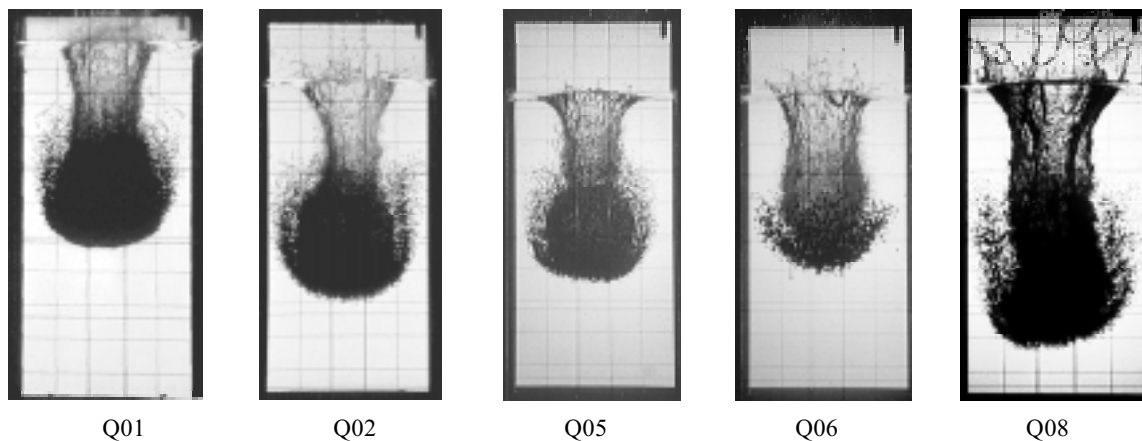
observations. The images of all the performed isothermal QUEOS premixing experiments are presented in Figure 3. Besides the simulated experiment Q08, experiments Q01, Q02, Q05 and Q06, where the spheres' diameter, spheres' material and spheres' total mass were varied, are also shown [11]. In all the images it is clear that the gas chimney starts to close in the middle, and not at the top as in the simulation.

To find out why the simulation results are qualitatively wrong a comprehensive parametric analysis was performed. Since the geometry of the model of experiment Q08, presented in [8], is not suited to a straightforward mesh-size-influence analysis, the parametric analyses were performed using a slightly different geometry (Figure 4). The spheres' jet radius



Sl. 2. Gostota združene faze voda - zrak, fazna verjetnost kroglic in hitrostno polje združene faze voda - zrak ob različnih časih pri simuliranju preskusa Q08

Fig. 2. The joint water-air phase density, the spheres' phase-presence probability and the joint water-air phase velocity field at different times during the simulation of experiment Q08



Sl. 3. Posnetki vseh izotermnih mešalnih preskusov QUEOS (posnetki vzeti iz [10])

Fig. 3. Images of all isothermal QUEOS premixing experiments (images taken from [10])

spremenjeni geometrijski obliki (sl. 4). Polmer curka kroglic smo zmanjšali z 9 cm na 8 cm in polmer posode z 41 cm na 40 cm. Tako so vse značilne dolžine modela večkrat deljive z 2, zaradi česar je parametrična analiza vpliva velikosti mreže lažje izvedljiva. Padajoče kroglice smo v model vključili z robnimi pogoji (RP), kar je opisano v [8].

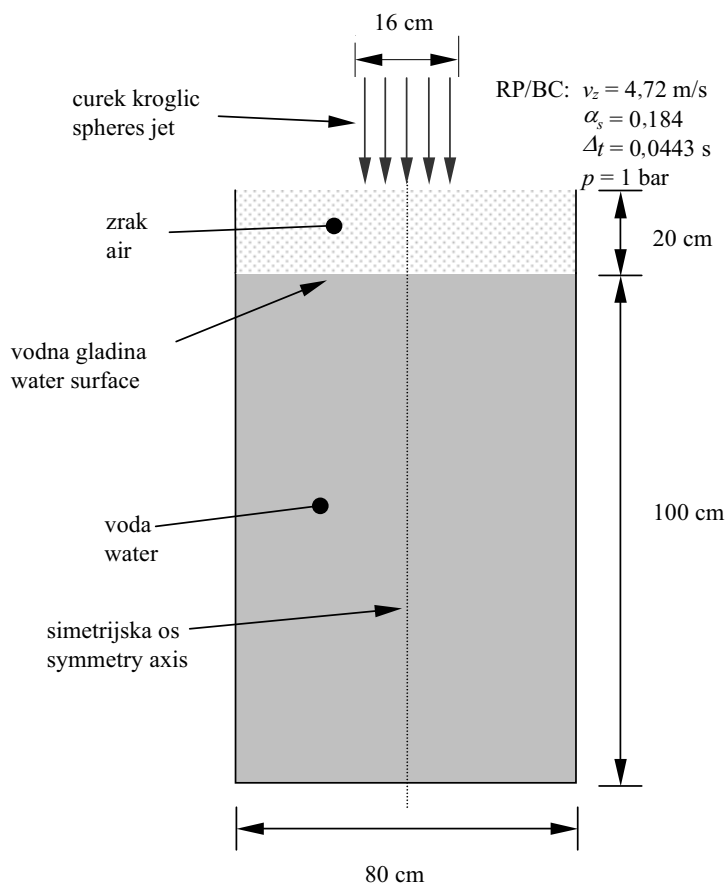
Najprej smo napravili analizo vpliva velikosti mreže, da bi ugotovili ali rezultati simuliranj konvergirajo k pravi fizikalni rešitvi. Kot osnovno mrežo, označeno z $1\times$, smo izbrali mrežo velikosti 40×120 točk. Tako je bila mrežna razdalja natančno 1 cm. Na sliki 5 so prikazani rezultati simuliranj, opravljenih na mrežah velikosti $0,5 \times (20 \times 60 \text{ točk})$, $1 \times (40 \times 120 \text{ točk})$ in $2 \times (80 \times 240 \text{ točk})$. Kakor je razvidno s slik, rezultati simuliranj ne konvergirajo k pravi fizikalni rešitvi, ampak prav nasprotno – z zgoščevanjem mreže postaja nefizikalno zapiranje plinskega stebra na vrhu še bolj izrazito.

Da bi ugotovili, ali je razlog za takšno obnašanje nefizikalni zvezni prehod zrak - voda v modelu zaradi reševanja enačb z metodo končnih razlik, smo simuliranja opravili pri različnih začetnih debelinah ε medfazne ploskve voda - zrak, pri čemer je ε določen z enačbo (3). Ker je pri metodi z nivojsko funkcijo debelina medfazne ploskve vnaprej določena in nespremenljiva za vse lege medfazne ploskve (tudi

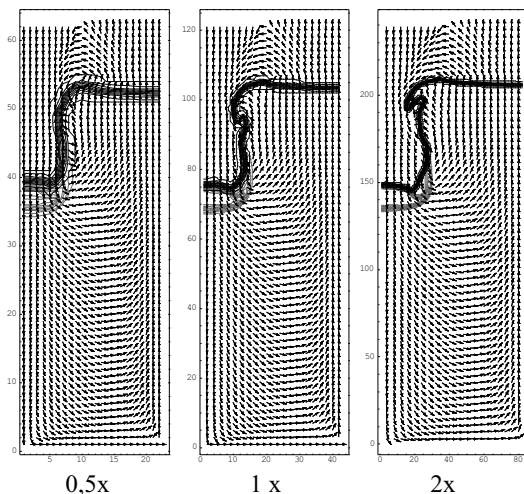
was reduced from 9 cm to 8 cm and the radius of the vessel from 41 cm to 40 cm. In this way all the characteristic dimensions of the model are more-times divisible by 2, which makes the mesh-size-influence analysis more straightforward. The falling spheres where introduced to the model with the boundary conditions (BC) as described in [8].

First the mesh-size-influence analysis was performed to establish whether the simulation results converge to the right physical solution. For the basic grid a mesh of 40×120 grid points, denoted with size $1\times$, was chosen. This meant that the grid spacing was exactly 1 cm. The results of the simulations performed on grid sizes $0.5 \times (20 \times 60 \text{ points})$, $1 \times (40 \times 120 \text{ points})$ and $2 \times (80 \times 240 \text{ points})$ are presented in Figure 5. As can be seen in the figure, the results do not converge to the right physical solution. On the contrary, with the finer mesh the unphysical closing of the gas chimney at the top becomes even more pronounced.

To find out if the reason for this behavior is the unphysical, gradual air-water transition in the model due to the numerical finite-differences solving procedure, the simulations were performed for different initial water-air surface thicknesses, ε , defined according to equation (3). Since for the level-set method the interface thickness is predetermined and constant for all interface positions (also vertical) this parametric analysis was performed



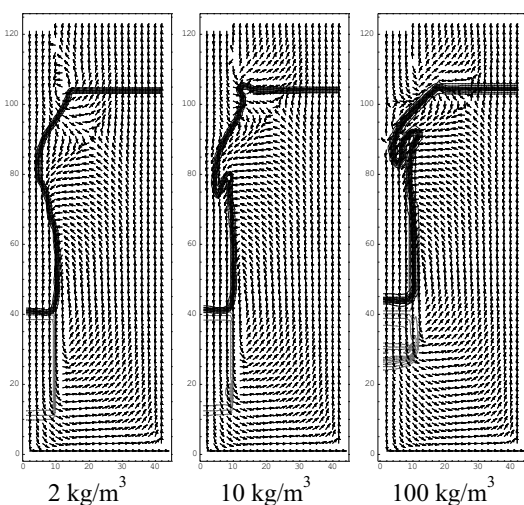
Sl. 4. Shema modela, prilagojenega za parametrično analizo
Fig. 4. Scheme of the model used for the parametric analyses



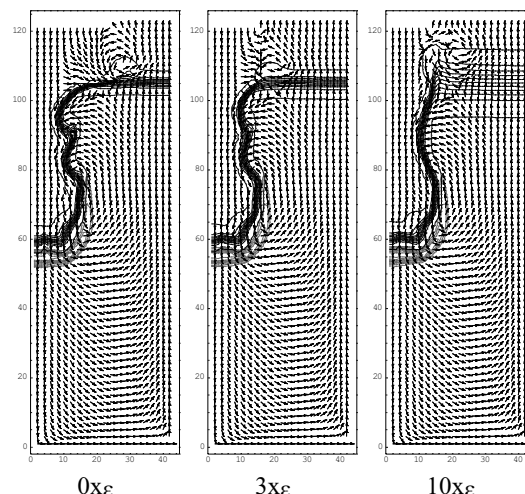
Sl. 5. Rezultati simuliranj pri času 610 ms, opravljeni na različno velikih mrežah
Fig. 5. The simulation results at time 610 ms performed for different mesh sizes

navpično), smo pri tej parametrični analizi gostoto združene faze voda - zrak določevali z metodo velike ločljivosti. Rezultati simuliranj, ki so prikazani na sliki 6, so presenetljivi in v nasprotju z našimi pričakovanji. Izkazalo se je, da se pri najbolj blagem prehodu zrak - voda začne zračni steber zapirati na pravem mestu v sredini, tako kakor pri preskusih.

Da bi pojasnili to nenavadno obnašanje, smo analizirali vpliv gostote vode na rezultate simuliranj. Na sliki 7 so prikazani rezultati simuliranj za različne umetne gostote vode. Vidimo, da se pri najmanjši gostoti vode 2 kg/m^3 , kar je le malo več od gostote zraka, začne zračni steber zapirati na sredini. To bi lahko bila razlaga, zakaj so rezultati pri najbolj blagem prehodu zrak - voda (sl. 6) kakovostno najboljši, saj je gostota združene faze voda - zrak v zgornji plasti



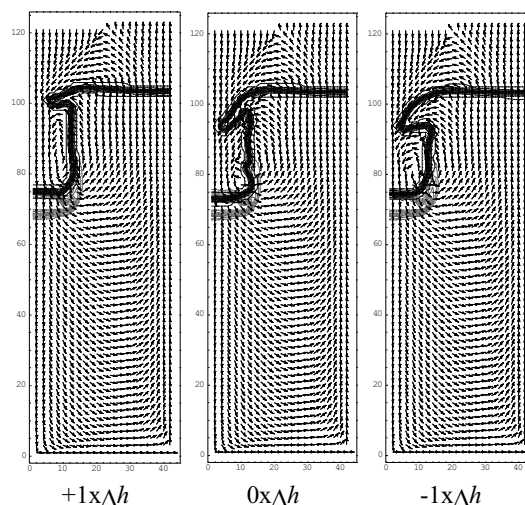
Sl. 7. Rezultati simuliranj pri času 660 ms za različne umetne gostote vode
Fig. 7. The simulation results at time 660 ms for different artificial water densities



Sl. 6. Rezultati simuliranj pri času 660 ms za različne začetne debeline medfazne ploskve voda - zrak
Fig. 6. The simulation results at time 660 ms for different initial water-air surface thicknesses

using the high-resolution method for the joint water-air phase-density determination. The results of the simulations, which are presented in Figure 6, are quite surprising, and the opposite of what we expected. It turned out that for the smoothest initial air-water transition the air chimney starts to close at the right place, in the middle, like the experimental observations.

To explain this strange behavior the influence of the water density on the simulation results was analyzed. The results of the simulations for different artificial water densities are presented in Figure 7. We can see that at the lowest water density, 2 kg/m^3 , which is only slightly higher than the air density, the air chimney starts to close in the middle. This could explain why the results for the smoothest air-water transition (Fig. 6) are qualitatively the best, since in the upper



Sl. 8. Rezultati simuliranj pri času 610 ms za različne lege vključitve sklopitve gibalne količine
Fig. 8. The simulation results at time 610 ms for different momentum-coupling starting positions

obsežne medfazne ploskve voda - zrak majhna in tako vrtinec nastane podobno kakor pri primeru z najmanjšo umetno gostoto vode (sl. 7).

Vendar, kaj je potem razlog za zapiranje zračnega stebra na vrhu? Dejansko je medfazna sklopitev gibalne količine kroglic med prostim padom skozi zrak precej majhna, potem pa se skokovito zveča, ko kroglice pričnejo prodirati v vodo. Da bi spoznali vpliv te skokovite spremembe medfazne sklopitve gibalne količine, smo napravili parametrično analizo, pri kateri smo sklopitev gibalne količine kroglic med prostim padom izklopili do določene globine. Rezultati simuliranj so prikazani na sliki 8. Medfazno sklopitev gibalne količine kroglic smo izklopili do ene mrežne razdalje nad vodno gladino ($+1 \times \Delta h$), do vodne gladine ($0 \times \Delta h$) in do ene mrežne razdalje pod vodno gladino ($-1 \times \Delta h$). Vidimo, da je zapiranje zračnega stebra na vrhu bolj izrazito, če je plast vode nad lego, kjer medfazna sklopitev gibalne količine kroglic prične vodo vleči navzdol, debelejša.

V modelu preskusa se lastnosti združene faze voda - zrak zaradi opisa s končnimi razlikami vedno spreminjajo postopoma in tako leži nad čisto fazo vode, kjer se medfazna sklopitev gibalne količine kroglic zveča na največjo vrednost, vedno neka prehodna plast z vmesno gostoto. Ta prehodna plast zaduši brizganje vode, ki se pojavi pri preskusih (sl. 3), in povzroči nefizikalno zapiranje zračnega stebra na vrhu (sl. 2). To zapiranje zračnega stebra je najizrazitejše na najgostejši mreži (sl. 5), kjer voda zaradi bolj podrobnega opisa ni več tako močno prisiljena k numerično odvisnemu kolektivnemu gibanju, debelina prehodne plasti pa je še vedno 1 cm.

Da bi odpravili to podedovano numerično pomanjkljivost modela, moramo v model vgraditi skokovito spremembo medfazne sklopitve gibalne količine kroglic na medfazni ploskvi zrak - voda, tako kakor je to dejansko, kar dosežemo s tem, da na skrajnem zgornjem območju prehodne plasti zrak - voda umetno povečamo medfazno sklopitev gibalne količine kroglic. To v praksi storimo najlažje tako, da v najvišji mrežni ravnini prehodne plasti zrak - voda, to je eno mrežno razdaljo Δh nad vodno gladino, medfazni koeficient trenja kroglic C pomnožimo z ustreznim faktorjem. Na sliki 9 so prikazani rezultati simuliranj, opravljenih z nespremenjenim ($1 \times C$) in pomnoženim koeficientom trenja kroglic ($10 \times C$, $20 \times C$). Kakor smo pričakovali, se začne zračni steber zapirati na pravem mestu v sredini, če v najvišji mrežni ravnini prehodne plasti zrak - voda koeficient trenja kroglic dovolj povečamo ($C^w \geq 10C$). Na sliki 11 je prikazan izračunani tlak v vodi, 250 mm nad dnom posode, za različne vrednosti koeficienta trenja kroglic C^w . S slik 11 in 9 je razvidno, da ima koeficient trenja kroglic v najvišji mrežni ravnini prehodne plasti zrak - voda zanemarljiv vpliv na rezultate simuliranj, če je dovolj velik ($C^w \geq 10C$). Zato smo v našem kombiniranem večfaznem

layer of the wide water-air interface the joint water-air phase density is low and so the vortex forms likewise in the lowest artificial water-density case (Fig. 7).

But why does the air chimney close at the top? In reality the spheres' momentum coupling during the free fall through the air is quite low and then abruptly rises when the spheres start to penetrate the water. To find out the influence of this abrupt momentum-coupling change a parametric analysis was performed, where the spheres' momentum coupling during the spheres' free fall was switched off until a certain depth. The results of these simulations are presented in Figure 8. The spheres' momentum coupling was switched off at one grid spacing over the water-air surface ($+1 \times \Delta h$), at the water-air surface ($0 \times \Delta h$) and at one grid spacing below the water-air surface ($-1 \times \Delta h$). It is clear that the air-chimney closing at the top is more pronounced if the water layer over the position, where the spheres' momentum coupling starts to drag the water down, is thicker.

In the experimental model the joint water-air phase properties always change gradually due to the finite differences' description and so there is always a transition layer with intermediate phases, density over the pure water phase, where the spheres' momentum coupling rises to its maximum value. This transition layer chokes the water splashing that is observed in the experiments (Fig. 3) and causes the unphysical air-chimney closing at the top (Fig. 2). This air-chimney closing at the top is most clearly demonstrated for the finest mesh (Fig. 5), where the water, due to the more detailed description, is not so strongly forced to the collective movement anymore, whereas the transition layer is still about 1-cm thick.

To overcome this inherent deficiency in the numerical model an abrupt increase in the spheres' momentum coupling at the water-air surface, as occurs in reality, has to be incorporated. This can be achieved if the spheres' momentum coupling at the upmost part of the air-water transition layer is artificially increased. This is most easily done if the spheres' interfacial drag coefficient C at the upmost mesh plane of the air-water transition layer, which is one grid spacing Δh over the water-air surface, is multiplied by a factor. The results of the simulations with the unmodified ($1 \times C$) and multiplied spheres' drag coefficient ($10 \times C$, $20 \times C$) are presented in Figure 9. As expected, the air chimney starts to close at the right place in the middle if the spheres' drag coefficient at the upmost mesh plane of the water-air transition layer is increased sufficiently ($C^w \geq 10C$). The calculated pressure in the water 250 mm above the bottom of the vessel is presented for different spheres' drag coefficients C^w in Figure 11. From Figs. 11 and 9 it is evident that the spheres' drag coefficient at the upmost mesh plane of the water-air transition layer has a negligible influence on the simulation results if it is large enough ($C^w \geq 10C$). So, in our

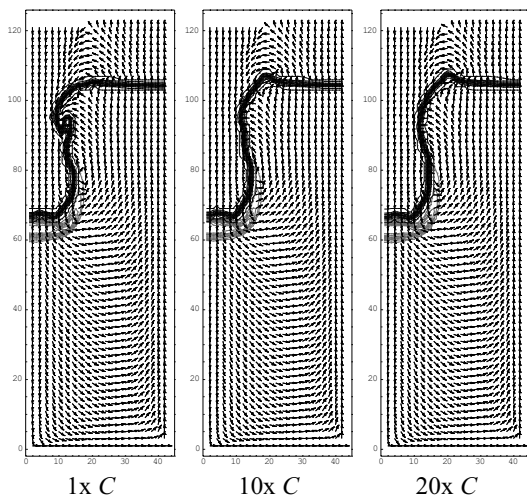
modelu za koeficient trenja kroglic v najvišji mrežni ravnini prehodne plasti zrak - voda vzeli naslednjo od velikosti mrežne razdalje odvisno vrednost:

$$C^{up} = 10 \frac{0,01m}{\Delta h} C \quad (5),$$

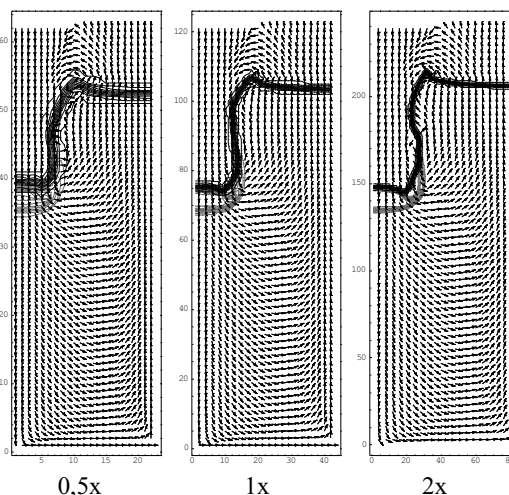
ki upošteva dejstvo, da je na gostejši mreži vpliv v eni mrežni ravnini povečanega koeficienta trenja kroglic manjši.

combined multiphase model at the upmost mesh plane of the water-air transition layer the following grid-dependent spheres' drag coefficient was chosen:

which takes into account the fact that on a finer grid the influence of the spheres' drag-coefficient increase in one mesh plane is lower.



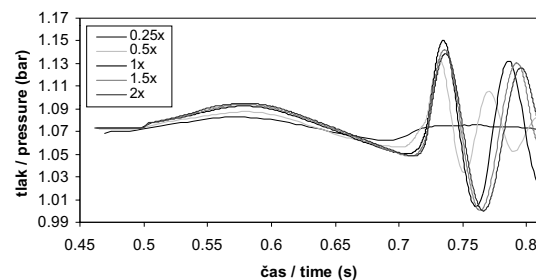
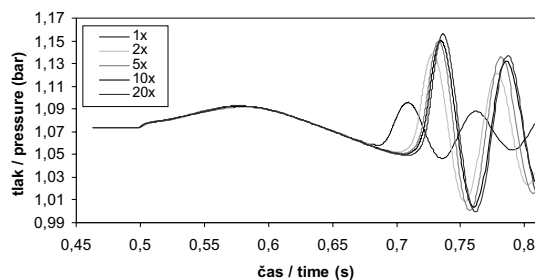
Sl. 9. Rezultati simuliranj ob času 635 ms za različne vrednosti koeficienta trenja kroglic v najvišji mrežni ravnini prehodne plasti zrak - voda
Fig. 9. The simulation results at time 635 ms for different spheres' drag coefficients at the upmost mesh plane of the water-air transition layer



Sl. 10. Rezultati simuliranj ob času 610 ms na mrežah različnih velikosti, opravljenih s spremenjenim koeficientom trenja kroglic
Fig. 10. The simulation results at time 610 ms performed with the modified spheres' drag coefficient on different mesh sizes

Na sliki 10 so prikazani rezultati simuliranj na mrežah različnih velikostih, opravljenih s spremenjenim koeficientom trenja kroglic (5). Vidimo, da se na vseh mrežah plinski steber razvije tako kakor v preskusih (sl. 3). Na sliki 11 so prikazane še tlačne krivulje, izračunane na mrežah različnih velikosti. Tlačne krivulje so sicer nekoliko odvisne od velikosti mreže tudi na gostejših mrežah (velikost mreže: 1x, 1,5x in 2x), vendar se to zgodi predvsem zaradi velike občutljivosti problema. Tako lahko sklepamo, da je osnovna mreža velikosti 1x z mrežno razdaljo 1 cm primerna za takšne vrste simuliranj.

The results of the simulations performed with the modified spheres' drag coefficient (Eq. 5) on different mesh sizes are presented in Figure 10. It is evident that the gas chimney develops like in the experiments (Fig. 3). The pressure curves calculated on different mesh sizes are presented in Figure 11. The pressure curves are also somewhat grid dependent on the finer meshes (mesh sizes: 1x, 1.5x and 2x), but that is mainly because of the very sensitive nature of the problem. We can conclude that the basic mesh size of 1x with the grid spacing of 1 cm is adequate for this type of simulation.



Sl. 11. Tlačne krivulje, izračunane za različne vrednosti koeficienta trenja kroglic C^{up} (leva stran) in na mrežah različnih velikosti (desna stran)

Fig. 11. Pressure curves calculated for different spheres' drag coefficients C^{up} (left-hand side) and on different mesh sizes (right-hand side)

Z razvitim kombiniranim večfaznim modelom z ustrezno spremenjenim koeficientom trenja kroglic v najvišji mrežni ravnini prehodne plasti zrak - voda (5) smo ponovno simulirali mešalni preskus Q08. Rezultati simuliranja so predstavljeni v prispevku [8].

4 SKLEP

Predstavili smo novo zasnovo obravnave večfaznih tokov, to je opis s kombiniranim večfaznim modelom, in jo preskusili na primeru izotermnega preskusa mešalne faze eksplozije pare. Ključna zamisel opisa večfaznega toka s kombiniranim večfaznim modelom je, da obravnavamo faze, ki ostanejo ločene s prosto površino (voda in zrak) z modelom proste površine kot eno, združeno fazo z nezveznimi faznimi lastnostmi, medtem ko preostale faze (kroglice) obravnavamo kakor običajno z modelom večfaznega toka. Stično površino (voda - zrak) določamo z nivojsko funkcijo, ki se v zadnjih letih veliko uporablja.

Z razvitim izvirnim kombiniranim večfaznim modelom smo simulirali mešalni preskus Q08, ki so ga izvedli na napravi QUEOS. Rezultati simuliranj so pokazali, da se plinski steber, ki nastane med prodiranjem kroglic v vodo, začne zapirati na napačnem mestu na vrhu stebra. Ugotovili smo, da pride od tega zaradi zvezne spremembe gostote na medfazni ploskvi voda - zrak v modelu preskusa, saj je nad čisto fazo vode zaradi opisa s končnimi razlikami vedno prehodna plast z vmesno gostoto. Ta prehodna plast zaduši brizganje vode, do katerega pride pri preskusih med prodiranjem padajočih kroglic v vodo, in povzroči nefizikalno zapiranje zračnega stebra na vrhu.

To podedovano numerično pomanjkljivost modela smo odpravili s posebno obravnavo medfaznega trenja kroglic na vodni gladini, na kateri smo koeficient trenja kroglic v najvišji mrežni ravnini prehodne plasti zrak - voda ustrezno povečali in tako dosegli skokovito spremembo medfazne sklopitve gibalne količine kroglic na medfazni ploskvi zrak - voda, tako kakor je to dejansko. Opravljena parametrična analiza je pokazala, da ima koeficient trenja kroglic v najvišji mrežni ravnini prehodne plasti zrak - voda zanemarljiv vpliv na rezultate simuliranj, če je dovolj velik. Tako smo lahko določili optimalno vrednost spremenjenega koeficienta trenja kroglic. Konvergenčna analiza je pokazala, da je mrežna razdalja 1 cm primerna za takšne vrste simuliranj.

Zahvala

Avtorji se zahvaljujejo Ministrstvu za šolstvo, znanost in šport, ki je finančno podprlo raziskavo v okviru raziskovalnega projekta Z2-3514.

With the developed combined multiphase model taking into account the modified spheres' drag coefficient at the upmost mesh plane of the water-air transition layer (Eq. 5) the premixing experiment Q08 was simulated once again. The results of the simulation were presented in the paper [8].

4 CONCLUSION

A new concept of multiphase flow treatment, the combined multiphase model formulation, was presented and applied to isothermal steam-explosion premixing experiments. The main idea of the combined multiphase model formulation is to treat the phases, which remain separated by a free surface (water and air), with a free-surface model as a single, joint phase with discontinuous phase properties, whereas the other phases (spheres) are treated, as is usual, with a multiphase flow model. The free surface (water-air) is determined with the front-capturing level-set method, which was widely used in recent years.

Using the developed, original, combined multiphase model the QUEOS isothermal premixing experiment Q08 was simulated. The simulation results showed that the gas chimney, which forms during the spheres' penetration into the water, starts to close at the wrong place at the top of the chimney. It was established that this happens because of the gradual change of the density at the water-air surface in the experimental model, since there is always a transition layer with intermediate phases' density over the pure water phase due to the finite differences' description. This transition layer chokes the water splashing observed in the experiments and causes the unphysical gas-chimney closing at the top.

This inherent deficiency of the numerical model was compensated with a special spheres' drag treatment at the air-water surface, where the spheres' drag coefficient at the upmost mesh plane of the water-air transition layer was appropriately increased and so an abrupt rise of the spheres' interfacial momentum coupling at the water-air surface, as occurs in reality, is achieved. The performed parametric analysis showed that the spheres' drag coefficient at the upmost mesh point of the water-air transition layer has a negligible influence on the simulation results if it is large enough. So, the optimum value of the modified spheres' drag coefficient could be established. The convergence analysis showed that a 1-cm grid spacing is appropriate for this kind of simulation.

Acknowledgment

The authors gratefully acknowledge the support of the Ministry of Education, Science and Sport of the Republic of Slovenia in the frame of the Research Project Z2-3514.

5 LITERATURA

5 REFERENCES

- [1] Černe, G., I. Tiselj, S. Petelin (2000) Upgrade of the VOF method for the simulation of the dispersed flow. *FEDSM 2000*, Vol. 251, New York, NY, CD-ROM.
- [2] Turland, B.D., G.P. Dobson (1996) Molten fuel coolant interactions: A state of the art report. European Commission, *Nuclear Science and Technology*, Luxembourg, ISSN 1018-5593.
- [3] Leskovar, M., J. Marn (1999) A combined single-multiphase flow formulation of the premixing phase using the level set method. *Nuclear Energy in Central Europe '99*, Portorož, Slovenija, Proceedings, 233-240.
- [4] Theofanous, T.G., W.W. Yuen, S. Angelini (1999) The verification basis of the PM-ALPHA code. *Nuclear Engineering and Design*, Vol. 189, 59-102.
- [5] Tiselj, I., G. Černe (2000) Some comments on the behaviour of the RELAP5 numerical scheme at very small time steps. *Nucl. sci. eng.*, Vol. 134, 306-311.
- [6] Leskovar, M., J. Marn, B. Mavko (2000) Numerical analysis of multiphase mixing – comparison of first and second order accurate schemes. *Fluid Mechanics Research*, Vol. 27, 1-32.
- [7] Marn, J., M. Leskovar (1996) Simulation of steam explosion premixing phase using probabilistic multiphase flow equations. *Fluid Mechanics Research*, Vol. 22 (1), 44-55.
- [8] Leskovar, M., B. Mavko (2002) Simuliranje izotermnega QUEOS preskusa mešalne faze eksplozije pare Q08. *Strojniški vestnik*, Vol. 48(2002)8, 449-458.
- [9] Sethian, J.A. (1998) Level set methods. *Cambridge University Press*, Cambridge.
- [10] Meyer, L., G. Schumacher (1996) QUEOS, a simulation-experiment of the premixing phase of a steam explosion with hot spheres in water, base case experiments. *FZKA Report 5612*, Forschungszentrum Karlsruhe.
- [11] Leskovar, M., J. Marn, B. Mavko (2000) The influence of the accuracy of the numerical methods on steam-explosion premixing-phase simulation results. *Journal of Mechanical Engineering*, Vol. 46, 607-621.

Naslov avtorjev: dr. Matjaž Leskovar
prof.dr. Borut Mavko
Institut "Jožef Stefan"
Jamova 39
1000 Ljubljana
matjaz.leskovar@ijs.si
borut.mavko@ijs.si

Authors' Address: Matjaž Leskovar
Borut Mavko
"Jožef Stefan" Institute
Jamova 39
1000 Ljubljana, Slovenia
matjaz.leskovar@ijs.si
borut.mavko@ijs.si

Prejeto:
Received: 6.8.2001

Sprejeto:
Accepted: 20.9.2002