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Title	A fluid interface model by phase field approach applied to the diffusive solution of level-set equation
Author(s)	OSHIMA, Nobuyuki
Citation	Mechanical Engineering Letters, 3, 17-00080-17-00080 https://doi.org/10.1299/mel.17-00080
Issue Date	2017-03-03
Doc URL	https://hdl.handle.net/2115/83859
Type	journal article
File Information	3_17-00080.pdf, Article



A fluid interface model by phase field approach applied to the diffusive solution of level-set equation

Nobuyuki OSHIMA *

*Faculty of Engineering, Hokkaido university
 Kita-13, Nishi-8, Nishi-ku, Sapporo, Hokkaido 060-8628, Japan
 E-mail: oshima@eng.hokudai.ac.jp

Received: 8 February 2017; Accepted: 26 February 2017

Abstract

Level-set approach extended for its diffusive solution is investigated to make a relation to conservation law of fluid phenomena and phase field approach based on the free energy theory. Considering mathematical analysis of level-set approach and re-initialization procedure, a new mathematical model of fluid interface is introduced defined by a cumulated layer of multiple contour elements. A generalized formulation of the extended level-set equation is derived by using phase field approach with a potential function model newly proposed for non-equilibrium solution of the local contour elements.

Key words : Level-set equation, Phase field approach, Conservation equation, Re-initialization procedure

1. A relation between the conservation law and the diffusive solution of level-set equation

Level-set approach is widely applied to interface problems in physical simulations (Osher et.al. 2002), and is also investigated as a powerful tool of mathematical analysis (Giga et.al. 2015). A concept of diffusive solution introduced by Chen et.al. (1991) confirmed a uniqueness for the solution of level-set equation. It leads to a basement of “re-initialization” procedure (Russo et.al. 2000, Olsson et.al. 2005) for suppressing numerical instability of the level-set equation. Ishida et.al. (2009) verified one-dimensional Allen-Cahn type equation, a most familiar model of phase field approach, to essentially the same solution. Using an analogy of the two interface models by the level-set and phase field approaches, Liu et.al. (2011) proposed a model for premixed combustion flame, and Oshima (2016) extended it to a three-dimensional formation for the diffusive solution of level-set equation.

Following to Liu and Oshima, a physical behavior of interface is considered by a relation to the scalar conservation law expressed by

$$\rho \frac{\partial \phi}{\partial t} = -\rho \mathbf{V} \cdot \nabla \phi + \nabla \cdot \mathbf{j} + \dot{q}. \quad (1)$$

Here a variable ϕ as the conservative scalar in fluid motived by the right hand side terms in the second formulation; the convection flux by material velocity \mathbf{V} and fluid density ρ , the diffusion flux by gradient model as $\mathbf{j} = D\nabla\phi$ (diffusion factor: D) and the source \dot{q} , respectively. When the variable ϕ changes from ϕ_- to ϕ_+ through the interface, the interface can be modeled as a cumulated layer of multiple contours (iso-surface) $\phi = \phi_0$ ($\phi_- \leq \phi_0 \leq \phi_+$) shown in fig.1. If each multiple contour has a continuous moving speed to the neighbors, it may form a “stable” interface where the local profile ϕ around the contour $\phi = \phi_0$ is identical to the level profile of ϕ_0 in the whole interface. It means that Eq.(1) gives the solution of level-set equation for any contour $\phi = \phi_0$ in the interface range ($\phi_- \leq \phi_0 \leq \phi_+$).

To derive the level-set formulation from the conservation equation (1), Liu introduced a local flame speed $s(\phi) = \dot{q} / |\nabla\phi|$ modeled by the linear function of ϕ , which describes both an interface propellant speed a steepness of the local solution by the level at the neutral position ($\nabla \cdot \mathbf{j} = 0$) and the gradient $\nabla\phi$, respectively. Oshima

combined her concept to Olsson's re-initialization procedure to derive the three-dimensional extension with both the normal propellant and curvature flows. They proposed an expected formulation derived from Eq.(1) as

$$\rho \frac{D\phi}{Dt} = \rho v(\phi, \nabla\phi) |\nabla\phi| + O(\phi, \nabla\phi) , \quad (2)$$

for the diffusive solution of level-set equation in fluid with considering. It means that a solution of Eq.(2) approximately satisfy the original level-set equation,

$$\frac{D\phi}{Dt} = v(\phi, \nabla\phi) |\nabla\phi| , \quad (3)$$

at the targeting contour under the condition to keep a continuous and monotonic profile in a neighbor thickness around the contour surface. Here the first term of the right hand side of Eq.(2) gives the motive force by the propellant speed v which corresponds to a local flame speed model by Liu et.al. and is defined by a traditional level-set approach at the interface element contour. The motive force, that is, propellant mass flux ρv should be generally a functional of ϕ and $\nabla\phi$, but in isotropic fluid can be modeled only by a propagation and curvature flow as

$$\rho v = s + c\kappa \quad (\text{normal flow factor: } s, \text{ curvature flow factor: } c \text{ and mean curvature: } \kappa) . \quad (4)$$

While the second term of Eq.(2) should converge to zero to describe a profile function of ϕ and $\nabla\phi$ which works as the re-initialization procedure at the interface area. By assuming the solution of profile function, the factors s and c become functions only by ϕ .

Though in the previous works by Liu and Oshima some possible formulations of Eq.(2) were derived and validated by numerical solutions for a simple combustion flame, their physical meaning has not been analyzed enough to apply extendedly to the generalized interface problems in more complicated conditions such as turbulence and detail chemistry, or in other physical phenomena such as gas-liquid interface of boiling bubbles and spray droplets. An empirical approach seems useless, because direct solutions or detail experiment data are unknown in the former cases, or a continuity assumption is even unavailable in the later ones.

So this paper asks a question what is a general law behind the similarity observed in those variety of interface problems, which can be widely applied to multi-physics and multi-scaled interface phenomena. Therefore it investigates a relation between the conservation law by Eq.(1) and the diffusive solution of the extended level-set approach by Eq.(2). A free energy theory may give a general law for the diffusion flux \mathbf{j} and source term \dot{q} of Eq.(1) as applied to a phase field approach for the interface phenomena, though it needs a little extension to non-equilibrium boundary condition at the local solution of the element contours by Eq.(2) instead of applying to equilibrium state by most of its previous researches. A new model for this purpose will be discussed in the next section.

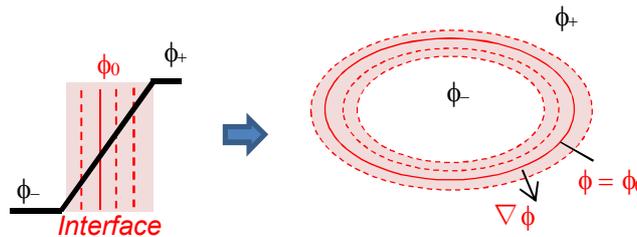


Figure 1 Level-set approach extended by a cumulated layer of multiple contours

2. A new functional formulation of phase field approach for the level-set diffusive solution

A phase field approach based on the free energy theory is applied for a formulation of the interface motive force in the level-set local solution described above. The phase field approach for interface problem is formulated by Euler-Lagrange equation,

$$\rho \frac{D\phi}{Dt} \equiv \rho \frac{\partial\phi}{\partial t} + \rho \mathbf{V} \cdot \nabla\phi = -M \sum \frac{\delta\Phi_i}{\delta\phi} , \quad (5)$$

by an order parameter ϕ which varies between the two phases around the interface. The variable ϕ corresponds to the level-set function indicating the contour for the interface position, too. Here considering the fluid phenomena by Eq.(1) or Eq.(2), a substantial derivative is introduced in the left hand side. In the right hand side, a functional value Φ_i defined as

$$\Phi_i = \int F_i dV, \tag{6}$$

by a free energy potential F_i describing the i -th elemental effect on the interface. In this research the potential functions are given by four components as

$$\begin{aligned} F_1 &= \int s(\phi)f(\phi)d\phi, \\ F_2 &= \frac{1}{2}\{f(\phi)\}^2, \\ F_3 &= \{d(\phi)-c(\phi)\}f(\phi)|\nabla\phi|, \\ F_4 &= \frac{1}{2}\{d(\phi)\}^2|\nabla\phi|^2. \end{aligned} \tag{7}$$

Here, F_2 and F_4 derive Allen-Cahn equation often applied to the phase field approach of the local equilibrium interface problems, and F_1 does its extended equation for non-equilibrium interface problems (Kobayashi 1993). F_3 is newly proposed by this paper for considering a local non-equilibrium near the element contour as discussed above, because the variable ϕ an element area bounded by its neighbor elements

In the phase field approach based on the fundament of thermodynamic theory, the minimizing of total functional value $\Sigma\Phi_i$ gives an equilibrium state by Eq. (5), where the variation of the functional is expressed as,

$$\begin{aligned} \frac{\delta\Phi_1}{\delta\phi} &= \frac{\partial F_1}{\partial\phi} = sf, \\ \frac{\delta\Phi_2}{\delta\phi} &= \frac{\partial F_2}{\partial\phi} = f\left(\frac{\partial f}{\partial\phi}\right), \\ \frac{\delta\Phi_3}{\delta\phi} &= \frac{\partial F_3}{\partial\phi} - \nabla \cdot \left(\frac{\partial F_3}{\partial\nabla\phi}\right) = \left(\frac{\partial(d-c)f}{\partial\phi}\right)|\nabla\phi| - \nabla \cdot ((d-c)f)\frac{\nabla\phi}{|\nabla\phi|} = -(d-c)f\kappa, \\ \frac{\delta\Phi_4}{\delta\phi} &= \frac{\partial F_4}{\partial\phi} - \nabla \cdot \left(\frac{\partial F_4}{\partial\nabla\phi}\right) = d\left(\frac{\partial d}{\partial\phi}\right)|\nabla\phi|^2 - \nabla \cdot d^2|\nabla\phi|\mathbf{n} \\ &= d|\nabla d||\nabla\phi| - d|\nabla\phi|(\nabla \cdot d\mathbf{n}) - d\mathbf{n} \cdot \nabla(d|\nabla\phi|) = -d^2|\nabla\phi|\kappa - d\mathbf{n} \cdot \nabla(d|\nabla\phi|) = -d\nabla \cdot d\nabla\phi \end{aligned} \tag{8}$$

$$\text{Unit vector normal to interface: } \mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}, \quad \text{Mean curvature: } \kappa = \nabla \cdot \mathbf{n}$$

Then

$$\sum \frac{\delta\Phi_i}{\delta\phi} = (s + f' + (c-d)\kappa)f - d\nabla \cdot d\nabla\phi, \quad f' = \left(\frac{\partial f}{\partial\phi}\right). \tag{9}$$

In the above derivation an identity of vector equations

$$\nabla \cdot f\mathbf{n} = |\nabla f| + f\kappa = f'|\nabla\phi| + f\kappa \quad \text{and} \quad \nabla \cdot d|\nabla\phi|\mathbf{n} = (d|\nabla\phi|)\kappa + \mathbf{n} \cdot \nabla(d|\nabla\phi|)$$

are used.

Here it is noted that the functional (6) is individually evaluated around each element contour, and that the mobility factor M in the Euler-Lagrange equation (3) is approximated by an inverse proportion of the thickness of integral volume of the functional (6). Now keeping a constant equivalent variation $d|\nabla\phi|$ in all the element integrations for deriving their common formulation, the integral thickness is estimated as a proportion to the factor d . Then assuming the mobility factor is given by $Md = 1$, the following equation is derived as

$$\rho \frac{D\phi}{Dt} = -(s + f' + (c-d)\kappa)\frac{f}{d} + \nabla \cdot d\nabla\phi. \tag{10}$$

Eq.(10) is identical to a non-equilibrium Allen-Cahn equation extended by Kobayashi (1993) with the interface

propellant mass flux $\rho v = s + c\kappa$ (see eq.(2)) instead of the propellant speed $v = (\rho v)/\rho$ of the interface element contour. It is also identical to a combustion flame model by Inage et.al (2000). The present formulation (10), however, allows any arbitrary coupling of the normal propellant and curvature flows (or to diminish them by $s = 0$ or $c = 0$), though the curvature flow wasn't explicitly considered but was implicitly included in the previous one by Kobayashi or Inage. Since the functional value is also expressed by

$$\sum \Phi_i = \int \left[\int s f d\phi - c f |\nabla \phi| + (f + d |\nabla \phi|)^2 \right] dV, \quad (11)$$

a trivial solution

$$\frac{f}{d} + |\nabla \phi| = 0 \quad (12)$$

gives its minimizing if $s = c = 0$. Here we can generally assume $d(\phi) > 0$ and $f(\phi) \leq 0$, $f(\phi) = 0$ at $|\nabla \phi| = 0$ by the condition that the equation (10) naturally connects to the bulk region ($|\nabla \phi| = 0$).

Using the solution (12), the right hand side of Eq.(10) is deformed as

$$RH = \rho v |\nabla \phi| - (\rho v + f') \left(\frac{f}{d} + |\nabla \phi| \right) + \nabla \cdot d \left(\frac{f}{d} + |\nabla \phi| \right) \mathbf{n}, \quad \rho v = s + c\kappa, \quad (13)$$

which gives a formulation of Eq.(2) for the diffusive solution of level-set equation. As Oshima analyzed, the last term of Eq.(13) has a role of re-initialization converging the thickness profile solution by Eq. (12) in the interface, and it is also expected that the second term, if $v = 0$, gives a converging solution around the contour surface at $f' = 0$. Such formulations were proposed by previous researches (Russo et.al. 2000, Olsson et.al. 2005) as the re-initialization procedures of the level-set equation. They are derived from the second and the third terms of Eq.(13) as follows;

Russo's formula:

$$-f = d = |\phi|, \quad \frac{\partial f}{\partial \phi} = -\text{sign}(\phi) \quad (\phi \neq 0) \quad \text{gives} \quad - \left(\frac{\partial f}{\partial \phi} \right) \left(\frac{f}{d} + |\nabla \phi| \right) = \text{sign}(\phi) (1 - |\nabla \phi|), \quad (14)$$

Olsson's formula:

$$f = \phi(\phi - 1), \quad \frac{\partial f}{\partial \phi} = 2\phi - 1, \quad d = 1 \quad \text{gives} \quad \nabla \cdot (f + d |\nabla \phi|) \mathbf{n} = \nabla \cdot (-\phi(1 - \phi) + |\nabla \phi|) \mathbf{n}. \quad (15)$$

Here the Olsson's formula satisfies the condition continuously connecting to the bulk region ($f(\phi) = 0$ at $|\nabla \phi| = 0$), but the Russo's formula diverges the variable ϕ linearly to the distance from the interface.

Finally assuming that a macroscopic solution of the global interface movement and a microscopic one of the local thickness profile are essentially independent, it is practically useful to introduce a modified solution of ϕ^* which can be more easily calculated by a coarse resolution for the macroscopic scale. This modification expresses a "thickened interface" (or "diffused interface") model in the present approach, which is easily formulated as

$$\rho \frac{\partial \phi}{\partial t} = (-\rho \mathbf{V} + \rho v \mathbf{n}) \cdot \nabla \phi - \left(\rho v + \frac{d}{d^*} f' \right) \left(\frac{f}{d^*} + |\nabla \phi| \right) + \nabla \cdot d \left(\frac{f}{d^*} + |\nabla \phi| \right) \mathbf{n}, \quad (16)$$

by introducing a constant factor $\frac{d}{d^*} > 1$. Eq.(16) keeps the same interface mass flux $\rho v = s + c\kappa$ in Eq.(11) and when the second and third terms disappear by the modified thickness profile

$$\frac{f}{d^*} + |\nabla \phi| = 0. \quad (17)$$

Eq.(16) is also expressed by a formulation of conservation law

$$\rho \frac{\partial \phi}{\partial t} + \rho \mathbf{V} \cdot \nabla \phi = \nabla \cdot \mathbf{j} + \dot{q}^*, \quad \text{where} \quad \mathbf{j} = d \nabla \phi \quad \text{and} \quad \dot{q}^* = - \left(s + \frac{d}{d^*} f' + (c - d) \kappa \right) \frac{f}{d^*}. \quad (18)$$

Here only the source term \dot{q}^* is modified form Eq.(10), which is essentially the same as a combustion flame model by Inage et.al. (2007) based on the phase field approach but includes the explicit effect of curvature flow. It should be

noted that a behavior of macroscopic interface movement is defined by the total phase change mass flux $\rho v = s + c\kappa$ and the convection and diffusion fluxes ($\rho \mathbf{V}$ and $\mathbf{j} = d\nabla\phi$) of background material flow, but isn't disturbed by the artificial large diffusion d^* only to avoid instability of the microscopic local solution in the interface thickness. It also makes clear an often discussed problem of the interaction between the macroscopic and microscopic interface modeling in the previous investigations (ex. Tiwari et.al. (2013), Gong et.al. (2015)). Eq. (18) is also available to apply for a turbulence diffusion model individually introduced from the interface propagation behavior.

3. Numerical results

In order to evaluate the fluid interface model proposed by the present work, a few of numerical solutions are introduced. In all cases Euler explicit scheme with a constant time increment and the second order central scheme with a uniform special grid are applied without any additional procedure. The density is set constant. Calculation conditions are expressed in table.1. At first one-dimensional steady propagation solutions by monotonic interface profiles are shown in fig.2. The original model by Eq.(10) and the thickened interface model by Eq.(16) with $d^* = 2d$ are solved from the same initial condition

$$\phi = \begin{cases} 0 & x < 0 \\ 0.5 & x = 0 \\ 1 & x > 0 \end{cases} \quad (19)$$

The both solutions shows a constant propellant speed given by the factor s because no curvature effect ($\kappa = 0$) appears in the one-dimensional monotonic profiles. The interface profiles are defined by Eq.(12) and Eq.(17) after the approaching time ($t > 0.5$) essentially independent to the initial profile, where the later solution with $d^* = 2d$ has a two-times thickness as the former one with d .

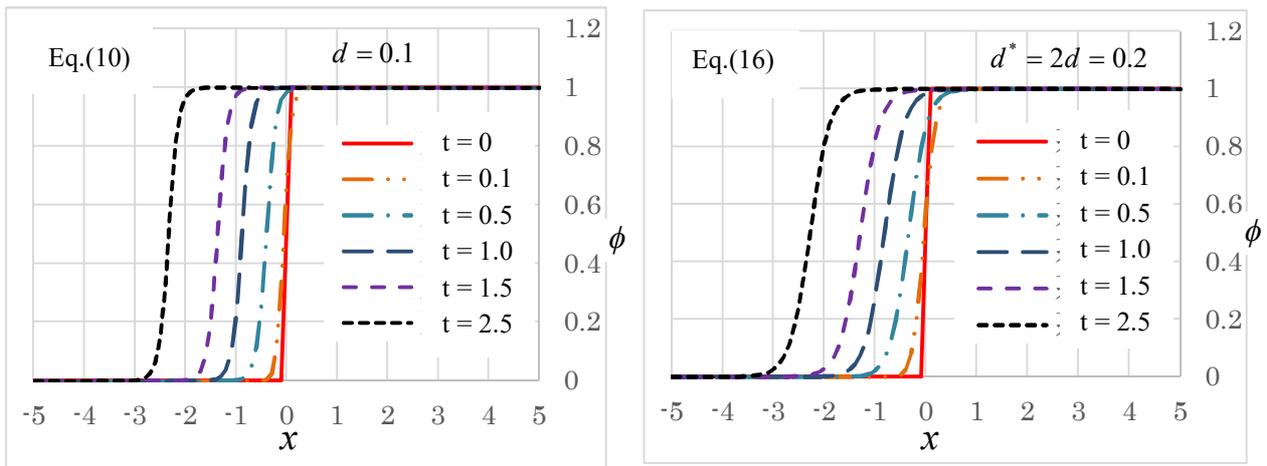


Fig.2 One-dimensional solutions of a monotonic single interface propagation by the original model eq.(10) and the thickened interface model eq. (16).

Table.1 Calculation conditions

	Monotonic solution	Non-monotonic solution	Axisymmetric solution
Time resolution	$\delta t = 0.01$		
Spatial resolution	$\delta x = 0.1$		
Outer boundary	$\frac{d\phi}{dx} = 0$ at $x = -5, 5$		$\frac{d\phi}{dr} = 0$ at $r = 5$
Propellant flow factor	$s = 1$	$s = 0$	$s = 0$
Curvature flow factor	-	$c = 0.2, 0$	$c = 0.25, 0$
Diffusion factor	$d = 0.1$ Eq.(10) $d^* = 0.2$ Eq.(16)	$d = 0.2$ Eq.(10)	$d = 0.25$ Eq.(10)

At next a non-monotonic initial profile shown in fig.3 is applied. For treating a singularity at the local minimum and maximum position numerically, the normal vector (one component) and the curvature on the discretized one-dimensional grid are defined as follows,

$$\mathbf{n} = \begin{cases} -1 & d\phi/dx < 0 \\ 0 & d\phi/dx = 0 \\ 1 & d\phi/dx > 0 \end{cases}, \quad \kappa = \begin{cases} -1/\delta x & \mathbf{n} = 0, \text{ local max.} \\ 0 & \mathbf{n} \neq 0 \\ 1/\delta x & \mathbf{n} = 0, \text{ local min.} \end{cases} \quad (20)$$

Since the singularity of normal vector doesn't appear in Eq.(10), the curvature at the local minimum or maximum position works to modify the initial profile. Therefore the traditional phase field model with the curvature flow effect implicitly ($c = d$ in Eq.(10)) by Kobayashi or Inage et.al. can't keep non-monotonic steady solution in the long time calculation, while the present model with no interface velocity condition ($\rho v = s + c\kappa = 0$) can hold a steady non-monotonic solution which becomes a diffusive solution of the original level-set equation (3) under the given initial profile appropriately.

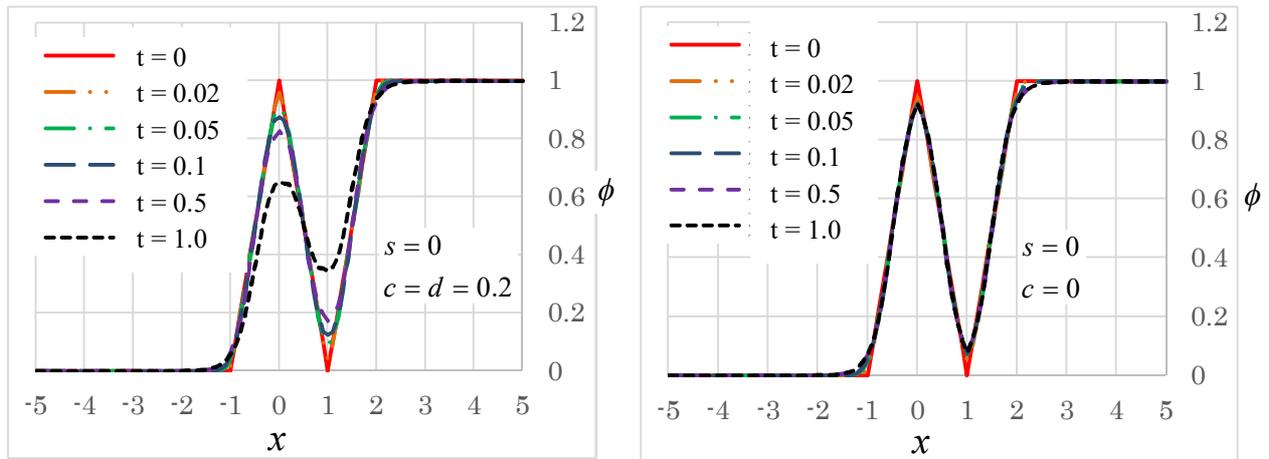


Fig.3 One-dimensional solutions of a non-monotonic interface with and without curvature flow ($\rho v = c\kappa$) by eq.(10).

Finally an example of multi-dimensional solution is shown in Fig.4, where Eq.(8) is applied to the axisymmetric isolated phase problem by the following initial profile

$$\phi = \begin{cases} 1 & r < r_0 \\ 0.5 & r = r_0, \quad r_0 = 1.5 \\ 0 & r > r_0 \end{cases} \quad (21)$$

In the axisymmetric coordinate the mean curvature is calculated by

$$\kappa = \frac{dn_r}{dr} + \frac{1}{r}, \quad \text{where a } r\text{-component of normal vector } n_r \text{ is defined as Eq.(20) } (x \rightarrow r), \quad (22)$$

The same treatment for the singularity is also applied at the local maximum in the center axis. Non-zero curvature flow

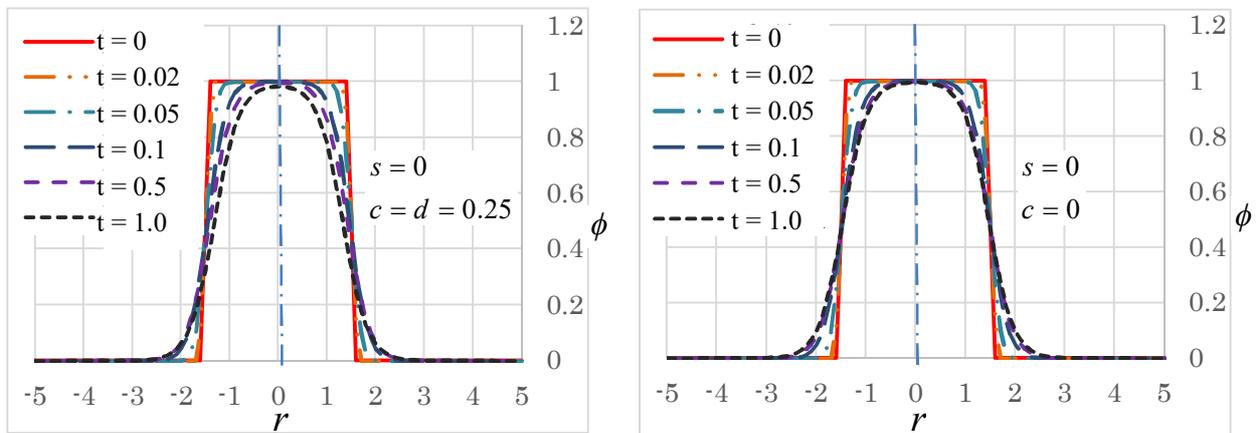


Fig.4 Axisymmetric solutions of an isolated phase with and without the curvature flow ($\rho v = c\kappa$) by eq.(10).

decreases a radius of the interface iso-surface ($\phi = 0.5$) and a volume of the inner phase region ($\phi > 0.5$). However no interface velocity condition ($\rho v = s + c\kappa = 0$) holds the initial interface position and the inner phase volume appropriately, though the interface profile converges to the target solution by Eq.(12) from the initial condition.

Now it should be noted again that all cases can be calculated without any upwind scheme, artificial diffusion or additional procedure for stabilizing numerical solution. It becomes an essential merit of the present formulation model for developing accurate solutions of complicated interface phenomena.

4. Conclusive remarks

This paper investigates the level-set approach extended for its diffusive solution to make a relation to conservation law of fluid phenomena and phase field approach based on the free energy theory. It leads to the two major proposals;

- 1) A new mathematical model of fluid interface is introduced defined by a cumulated layer of multiple contour elements;
- 2) A generalized formulation of the extended level-set equation is derived by using phase field approach based on the free energy theory with a potential function model newly proposed for non-equilibrium solution of the local contour elements.
- 3) A formulation by the differential equations with an explicit and conservative diffusion term able to apply a simple numerical method without any stabilizing artificial procedure such as an upwind scheme or an additional re-initialization. They are also available to investigate a mathematical fundament of the thickened interface model and the averaging turbulence model.

Acknowledgement

This research was supported by JSPS KAKENHI Grant Number 15H3912.

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