DS Journal of Modeling and Simulation
Volume 3 Issue 2, 1-9, Apr - Jun 2025
ISSN: 2584-1564 / https://doi.org/10.59232/MS-V3I2P101

Original Article

Numerical Modeling of Coefficient of Surface Tension at Fluid Gas Interface

M. Shoikhedbrod[1*], I. Shoikhedbrod[1]

[1]*R&D Department of Electromagnetic Impulse Inc., 21 Four Winds Drive, Unit 12, North York, Ontario, M3J 1K7, Canada.*

*michaelshoikhedbrod@bell.net

Received: 04 February 2025; Revised: 03 March 2025; Accepted: 02 April 2025; Published: 30 April 2025

Abstract - Among the known experimental and theoretical methods for calculating the coefficient of surface tension at the boundary of liquid-gas phases, the most suitable is the technique used by F. Bashforth and J. Adams, applying tables for calculating profiles of dimensionless drops, compiled from photographs of existing liquid drops of a wide diapason of numbers of Bond and edge angles of wetting by hand. The tables, compiled by this technique, were exchanged in many articles on computer calculations of the shapes of dimensionless drops. These computer calculations duplicated these tables, and in connection with this, the determination of the Bond number, at least approximately, of the corresponding liquid drop, was carried out manually, which led to the fact that the calculation of the liquid drop profile was far from the real image of the liquid drop in the photograph, and, accordingly, an accurate calculation of the coefficient of surface tension at the boundary of liquid-gas phases became impossible. The author proposed a newly developed method for the accurate numerical modeling of the coefficient of surface tension at the boundary of liquid-gas phases of a drop of liquid based on photographs of a real drop of liquid, in which the Bond number was adjusted to the corresponding Bond number of a real drop of liquid automatically by a computer with high accuracy, which made it possible to accurately numerically model the coefficient of surface tension at the boundary of liquid-gas phases of a drop of liquid, the profile of which coincided with high accuracy with the photo image of the shape of a real drop within a few seconds. The article presents a computer program, written in the Turbo Basic computer language, compiled by the algorithm of a previously developed model, which makes it possible to accurately numerically model the coefficient of surface tension at the boundary of liquid-gas phases of a drop of liquid, the profile of which coincided with a high accuracy with the photo image of the shape of a real drop, and display the calculation results of the model on the computer screen within a few seconds.

Keywords - The coefficient of surface tension, Boundary of liquid-gas phases, Drop image, Computer numerical modeling, Bond numbers.

1. Introduction

There are the following experimental techniques for the determination of the coefficient of surface tension at the boundary of liquid-gas phases: the pressure technique, the technique using the mass of the drop of fluid, Wilhelm's technique (weighing method) and Laplace's method [1-3]. However, all these methods require accurate measurements on special equipment, which makes calculating the surface tension coefficient rather inaccurate. Among the known experimental and theoretical methods for calculating the coefficient of surface tension at the boundary of liquid-gas phases, the most suitable is the technique used by F. Bashforth and J. Adams, applying tables for calculating profiles of dimensionless drops compiled from photographs of existing liquid drops of a wide diapason of numbers of Bond and edge angles of wetting by hand. In many articles, these tables were exchanged for computer calculations of the shapes of dimensionless drops.

These computer calculations simply duplicated these tables, and in connection with this, the determination of the Bond number, at least approximately, of the corresponding liquid drop, was carried out manually, which led to the fact that the calculation of the liquid drop profile was far from the real image of the liquid drop in the photograph, and, accordingly, an accurate calculation of the coefficient of surface tension at the boundary of liquid-gas phases became impossible.

Thus, the main disadvantage of the above techniques is the impossibility of obtaining a highly accurate calculation of the surface tension coefficient at the boundary of liquid-gas phases. The task arises of creating a technique that allows one to easily calculate the coefficient of surface tension at the boundary of liquid-gas phases with high accuracy.

The paper presents a newly developed technique of the accurate numerical modeling of the coefficient of surface tension at the boundary of liquid-gas phases of a drop of liquid, based on photographs of an existing drop of liquid, in which the number of Bond was adjusted (modeling) to the corresponding number of Bond of an existing drop of liquid automatically by a computer with assigned high accuracy, which made it possible to accurately numerically model the coefficient of surface tension at the boundary of liquid-gas phases of a drop of liquid, the profile of which coincided with an assigned high accuracy with the photo image of the shape of a exist drop within a few seconds.

The scientific novelty of the developed technology is the adjustment of the Bond number (modeling) to the corresponding Bond number of an existing drop of liquid with a given high accuracy automatically, using a computer, within a few seconds, with a given accuracy, to numerically model the coefficient of surface tension at the boundary of liquid-gas phases of a drop of liquid, the profile of which coincides with a given accuracy with a photo image of the shape of an existing drop.

2. Materials and Methods

For example, a photo of drop water on a glass surface was taken. In [6], a block - scheme of an algorithm for numerical modeling of Bond numbers for a wide range of liquid droplets based on photographs of real liquid droplets, in which the selection of the number of Bond corresponding to an existing liquid droplet is performed automatically by a computer with high accuracy, which allows for the coefficient of surface tension at the boundary of liquid-gas phases to be numerically modeled with high accuracy within a few seconds. The scheme of the algorithm, presented in Figure 1 [6], includes the following operations:

1. Input of initial data: ρ_{fl}- fluid density; g - acceleration due to gravity, B - any number close to the calculated parameter: Bond Number - β; F = 1.5708 radians - angle equal to 90˚; σ_{12}= T is the coefficient of surface tension at the boundary of liquid-gas phases (for determination of the value of β and the normalizing coefficient $\boldsymbol{b}$, an experimentally set bubble profile is used); AC - X / Z ratio at F = 90˚, which is determined experimentally from the photo (Figure 2, [6]); DI is the radius of the cross-section of bubble shape at the point F = 90˚, which is determined experimentally (for the determination of the coefficient of surface tension at the boundary of liquid-gas phases, the experimentally assigned bubble profile is used); A4- the accuracy of the adjustment of the computable value $A = \frac{X}{Z}$ to AC; D - the step of increment by B. In a computer program of numerical modeling of the value of the coefficient of surface tension at the boundary of liquid-gas phases and the normalizing coefficient of a bubble (drop), if its shape (drop) is set experimentally (in the form of a photo), fixed on the solid surface in a liquid, written in computer language Turbo Basic, the input data is entered as follows:

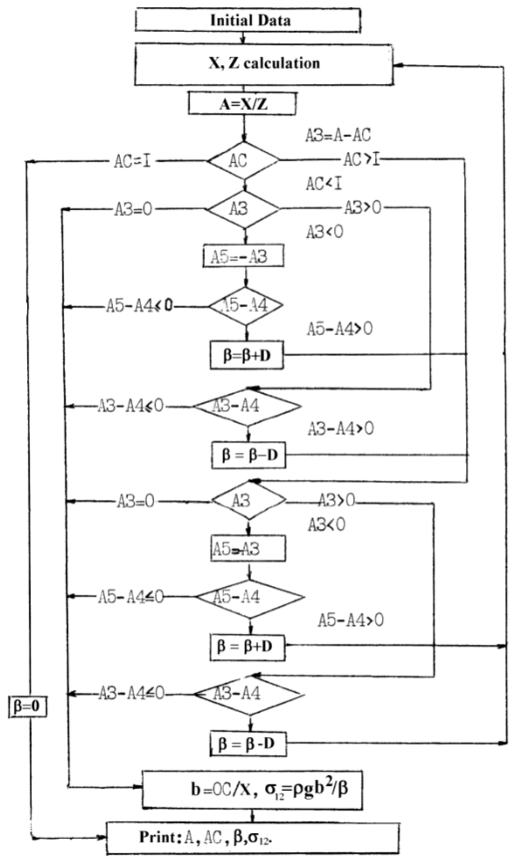

Fig. 1 Block - schema of the algorithm of numerical modeling of the bond number, coefficient of the surface tension (σ_{12}) and normalizing factor of gas bubble from experimentally assigned profile of its form

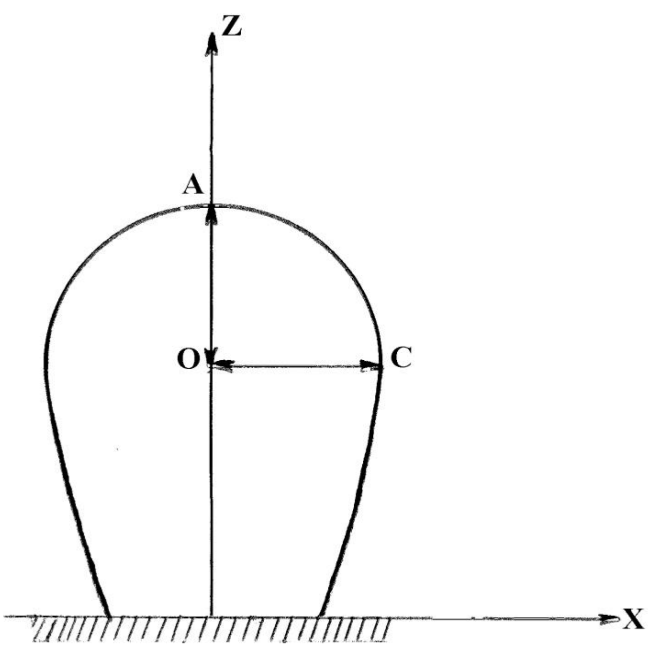

Fig. 2 Drop of fluid (gas bubble) on the solid surface.
OC - the coordinate X of the form of the drop with F= 90˚;
OA - the coordinate Z of the form of the drop with F = 90˚

91 LOCATE 25,42:INPUT "For continue, press ENTER ", T10

```
95 CLS: lux=1: luy=1: h=8: d=68: c=9: gosub 2150
97 locate 2, 2: color 14, 0: PRINT “G0 - earth accelerate; P0 - liquid density; T0 - any surface tension”
98 locate 3,2:PRINT " B0 - any multiplicate number."
100 color 15,0:locate 4,2:PRINT " AP=AC/OA - X and Z relation at agle point F=90 (from picture)"
125 locate 5,2:PRINT” DI- X coordinate -AC (from picture).”
150 color 10:locate 6,2:PRINT “ZN - Bond Number sign.”
155 locate 7,2:PRINT " If ZN=1 Bond Number >O,if ZN < 0, Bond Number < 0."
180 rem
190 locate 10,2:color 7,0:INPUT "Enter parameters G0(980),P0(1),T0(190)...",G0,P0,T0
192 LOCATE 11,2:INPUT "Enter parameters AP(1.65), DI(0.58), B0(1), ZN(1)...", AP0,DI0,B0,ZN
```

The printout of the program’s entered data on the computer screen is represented in Figure 3.

2. The values of coordinates ***X***, ***Z*** and relation ***X/Z*** at ***F =90***$^{\circ}$ for the randomly given number ***B*** are calculated.

3. It produces a comparison and then the adjustment of the value of the calculated relation X/Z to the value AC by increasing the initially given number B.

This operation provides three cases:

Case 1. AC = 1, which corresponds to B = 0.

In this case, the values AC = 1, B = 0 will be printed.

Case 2. AC > 1, which corresponds to B > 0.

In this case, the following actions are carried out:

a) if the calculated relation $A=\frac{X}{Z}$ is more than the compared value *AC*, then with the assigned accuracy, *A4* is produced adjustment *A* to *AC* by decreasing the given value *B* with the step of *D* until *A* and *AC* coincide with the accuracy *A4*. After this, when *A* = *AC*, the value *B* is substituted to the formula for determination of the *AC* = *AP* = *AC/OA*, which is determined by the photograph (Figure 3).

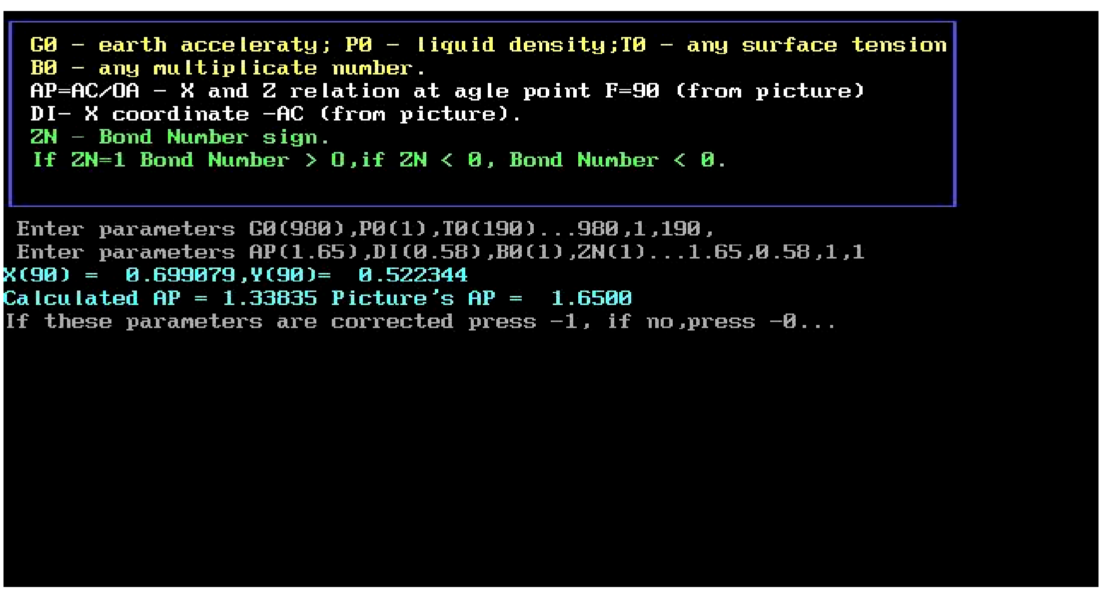

Fig. 3 Printout of the program data input on the computer screen

Normalizing Factor *B1*:

$$B1 = \sqrt{\frac{BT}{\rho g}} \qquad (1)$$

and formula for determination of the coefficient of surface tension at the boundary of liquid-gas phases:

$$T2 = \frac{1}{B}\rho_{fl} g \left(\frac{DI}{X}\right)^2, \text{ at } F = 90^{\circ} \qquad (2)$$

b) if $A = \frac{X}{Z}$ is less than the value AC, then with the accuracy $A4$ is produced adjustment A to AC increases the given value B with a step of D until A and AC coincide with the accuracy $A4$. Further operations are analogous to the actions of point (a).

Case 3. AC < 1, which corresponds to B<0.

In this case, the following actions are carried out:

a) If $A = \frac{X}{Z}$ is more than value AC, then with the accuracy $A4$ is produced adjustment A to AC by decreasing the given value B with a step of D until A and AC coincide with the accuracy $A4$. The remaining operations are analogous to the actions of case 2.

b) If $A = \frac{X}{Z}$ is less than the value AC, then further operations are performed analogously to the actions of the case 2 point (b).

The original code of the developed program, written on computer language Turbo Basic, operating by the above-described algorithm of precise modeling of the coefficient of surface tension at the boundary of liquid-gas phases and the normalization factor is as follows:

```
240 TB=1.E-10:C(1)=1.E-10:C(2)=1.E-10:C(3)=TB:TB=3.1416/NI
250 GOSUB 1190
255 B10=P*G*(B^2)/T
260 X1(1)=C(1):ZO=C(1)/C(2)
270 AO=ZO-AP
280 PRINT “Calc.AP = ";:PRINT USING "##.####" ;ZO;:PRINT ",  Picture AP = ";:PRINT USING "##.####"; AP;
281 PRINT ",  Bond Number = ";:PRINT USING "####.####"; B10
290 IF AO=0 THEN 460
300 IF AO>0 THEN 390
310 AO=-AO
320 IF AO-DH<=0 THEN 460
330 IF ZN<0 THEN 370
340 IF B=0 THEN 460
350 B=B+DB
360 GOTO 240
370 B=B+DB
380 GOTO 240
390 IF AO-DH<=0 THEN 460
400 IF ZN<0 THEN 440
410 IF B=0 THEN 460
420 B=B-DB
430 GOTO 240
440 B=B-DB
450 KS=KS+1
```

```
455 GOTO 240
460 BO=(P*G*(B^2))/T
470 B1=DI/X1(1)
480 T1=(P*G*(B1^2))/BO
490 CLS:lux=1:luy=1:h=3:d=50:c=9:gosub 2150:locate 2,2:COLOR 7: PRINT” AC/OZ relation by picture, calculated relation”
500 locate 3,2:color 14:PRINT USING "      ####.####              ####.####"; AP,ZO
510 lux=1:luy=5:h=3:d=50:c=12:gosub 2150:locate 6,2:COLOR 7:PRINT " Mult.number,  Bond Number,  Surface Tension”
520 locate 7,2:COLOR 14:PRINT USING "  ####.####     ####.####      ####.####"; B1,BO,T1:
530 locate 25,42:COLOR 7,0:INPUT “For continue, press ENTER”,T10:CLS
1169 GOTO 70
1170 STOP
1180 END
1190 REM INITIAL DATA FOR SUBROUTINE KMRSNA INPUT
1200 X=TB:XEND=TE:H=.001:EP=.000001
1210 GOSUB 1230
1220 RETURN
1230 REM SUBROUTINE KMRSNA
1240 HP=ABS(XEND-X):X0=X:FOR I=1 TO NC:Y0(I)=C(I):NEXT I
1250 PLO=1:FF$= “TRUE”
1260 IF PLO>=ABS(HP/H) THEN 1280
1270 PLO=2*PLO:GOTO 1260
1280 H=HP/PLO
1290 LO=0
1300 X=X0
1310 FOR I=1 TO NC:C(I)=Y0(I):NEXT I
1320 GOSUB 1670
1330 X=X0+H/3.:FF$= “FALSE”
1340 FOR I=1 TO NC:F0(I)=Z(I):C(I)=Y0(I)+H*Z(I)/3.:NEXT I
1350 GOSUB 1670
1360 FOR I=1 TO NC:C(I)=Y0(I)+(F0(I)+Z(I))*H/6.:NEXT I
1370 GOSUB 1670
1380 X=X0+H/2.
1390 FOR I=1 TO NC:F1(I)=Z(I):C(I)=Y0(I)+(F0(I)+3.*Z(I))*H/8.:NEXT I
1400 GOSUB 1670
1410 X=X0+H
1420 FOR I=1 TO NC:F2(I)=Z(I):C(I)=Y0(I)+(F0(I)-3.*F1(I)+4.*Z(I))*H/2.
1430 Y1(I)=C(I):NEXT I
1440 GOSUB 1670
1450 FOR I=1 TO NC:Y2(I)=Y0(I)+(F0(I)+4.*F2(I)+Z(I))*H/6.:NEXT I
1460 INC$= “TRUE”
1470 FOR I=1 TO NC:BBB=ABS(.2*(Y1(I)-Y2(I))):ER1=ABS(Y1(I))
1480 IF BBB>ER1*1E-18 THEN 1490
1490 IF BBB*1E-18<ER1 THEN 1510
1500 ER1=BBB:GOTO 1520
1510 ER1=BBB/ER1
1520 IF ER1<=EP THEN 1540
```

```
1530 H=H/2.:PLO=2.*PLO:LO=2*LO:GOTO 1300
1540 IF ER1*65.>EP THEN INC$="FALSE"
1550 NEXT I
1560 FF$= "TRUE":X0=X0+H
1570 FOR I=1 TO NC:Y0(I)=Y2(I):NEXT I
1580 LO=LO+1
1590 IF LO<PLO THEN 1630
1600 X=X0
1610 FOR I=1 TO NC:C(I)=Y0(I):NEXT I
1620 RETURN
1630 IF INC$= "TRUE" THEN 1640
1640 IF LO=(LO/2)*2 THEN 1660
1650 GOTO 1300
1660 H=2.*H:LO=LO/2:PLO=PLO/2:GOTO 1300
1670 REM CALCULATION OF DIFFERENTIAL EQUATION
1680 A9=C(3)
1690 IF KC-1>=0 THEN 1730
1700 P1=P*G*C(2)*(B^2)/T
1710 IF ZN<0 THEN P1=P1*(-1)
1720 P2=SIN(A9)/C(1):D0=1./(2.+P1-P2):D1=D0
1730 Z(1)=D0*COS(A9):D0=D1:Z(2)=D0*SIN(A9):Z(3)=1.
1740 RETURN
```

3. Results and Discussion

The comparison and then the adjustment of the value of the calculated ratio Calc.AP = A = $\frac{X}{Z}$ to the value of Picture AP =AC ($\frac{AC}{OA}$) by the increase of the initially given number *B* if the calculated relation A= $\frac{X}{Z}$ is more than the compared value AC on the printout of the program on the computer screen (Figure 4, [6]).

Figure 5, [6] presents the printout of the results of the work of the program on the computer screen: the relation of Picture AP =AC ($\frac{AC}{OA}$) on Figure 2 and the calculated relation Calc. AP = A = $\frac{X}{Z}$; the calculated values of normalizing factor *B0(b)*; the Bond number B (β) and the coefficient of surface tension at the boundary of liquid-gas phases T2 (σ_{12}) of the gas bubble Time of calculation of program on the personal computer comprises less than the minute.

Thus, the developed computer program, written in the Turbo Basic computer language, compiled by the algorithm of a previously developed model, which makes it possible to accurately numerically model the coefficient of surface tension at the boundary of liquid-gas phases and normalizing factor of the bubble (drop) of wide diapason range of numbers of Bond, the profile of which coincides with high accuracy with the photo image of the exist profile bubble (drop) and display the results of the modeling on the computer screen for a few seconds.

4. Conclusion

Thus, the presented computer program, written in Turbo Basic computer language, compiled by the algorithm of the developed model, which makes it possible to accurately numerically calculate the coefficient of surface tension at the boundary of liquid-gas phases and normalizing factor of bubble (drop) of wide diapason of numbers of Bond, the profile of which coincides with a high.

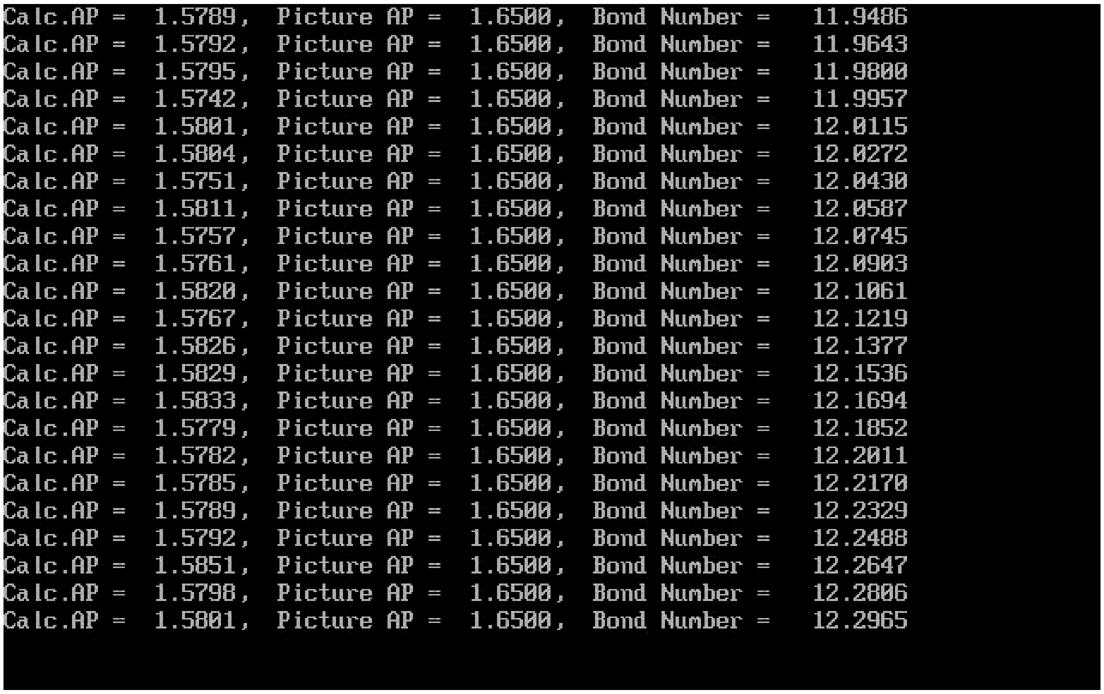

Fig. 4 Printout of comparison, and then the adjustment of the value of the calculated ratio *Calc.* AP =A = X/Z to the value *Picture* AP = AC (AC/OA) (on the Figure 1) = 1.6500 radians with the accuracy A4 = 0.01 by the increase of the initially given number B (β) on the computer screen

Fig. 5 Printout of the results of the work of the program on the computer screen:
a) Relation *AC* = *AP* = *(AC/OA)* on the photograph (Figure 1) and calculated relation A=X/Z at F = 90˚,
b) The calculated value of normalizing factor B0 (b),
c) The calculated value of the number of Bond B (β), and
d) The calculated value of the coefficient of surface tension *T2* (σ_{12}) of the gas bubble on the border of the phase section of liquid gas.

Accuracy with the photo image of the existing profile bubble (drop) and display the modeling results on the computer screen for a few seconds.

References

[1] E.A. Shimko et al., “Methods of Surface-Tension Experimental Evaluation”, "Izvestiya of Altai State University Journal, vol. 1, no. 89, pp. 1-15, 2016. [CrossRef] [Publisher Link]

[2] Franco Emmanuel Benedetto, Hector Zolotucho, and Miguel Oscar Prado, “Critical Assessment of the Surface Tension Determined by the Maximum Pressure Bubble Method”, Materials Research, vol. 18, no. 1, pp. 9-14, 2015. [CrossRef] [Google Scholar] [Publisher Link]

[3] Boon-Beng Lee, Pogaku Ravindra, and Eng-Seng Chan, “A Critical Review: Surface and Interfacial Tension Measurement by the Drop Weight Method,” Chemical Engineering Communications, vol. 195, no. 8, pp. 889-924, 2008. [CrossRef] [Google Scholar] [Publisher Link]

[4] Francis Bashforth, and J.C. Adams, Capillary Action, Cambridge University Press Warehouse, London, 1883. [Publisher Link]

[5] M.A. Ponomareva, and V.A. Yakutenok,“Method of determination the coefficient of surface tension and wetting angle on the image of the drop,” *Fluid and Gas Mechanics : Bulletin of the Nizhny Novgorod University Named After N.I. Lobachevsky*, vol. 4, no. 3, pp. 1048-1049, 2011. [Publisher Link]

[6] Michael Shoikhedbrod, “Method of Determination of the Coefficient of the Surface Tension on the Drop Image Using the Computer Mathematical Modeling”, International Journal of Chem-Informatics Research, vol. 5, no. 2, pp. 1-8, 2019. [Google Scholar] [Publisher Link]