Applicability of submerged jet model to describe the liquid sample load into measuring chamber of micron and submillimeter sizes

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Abstract. The load of a liquid sample into a measuring chamber is one of the stages of substance analysis in modern devices. Fluid flow is effectively calculated by numerical simulation using application packages, for example, COMSOL MULTIPHYSICS. In the same time it is often desirable to have an approximate analytical solution. The applicability of a submerged jet model for simulation the liquid sample load is considered for the chamber with sizes from hundreds micrometers to several millimeters. The paper examines the extent to which the introduction of amendments to the jet cutting and its replacement with an energy equivalent jet provide acceptable accuracy for evaluation of the loading process dynamics.

1. Introduction
Mass transfer in laminar flow with transverse Reynolds numbers less than 1 is often used during the liquid injection from a channel with small cross-section to a large tank in devices for the analysis of liquid samples. Understanding the dynamics of the input is very important, as a chemical reaction starts at the moment of the sample load in a number of analytical schemes [1]. If measuring chamber has an aspect ratio (diameter/depth) of 10 or more, submerged jet scheme can be applied only at the initial stage, when the expanding jet is entirely placed within the chamber boundaries. Otherwise, the jet will be "cut" in the vertical plane. This effect can be taken into account. When the liquid front becomes close to the chamber wall, the fundamental limitation of the model - the principle of momentum flux conservation - breaks down by the addition of the momentum reflected from the wall. The problem of the jet dynamics into a submerged space strictly mathematically formulated and solved as a first approximation by L.D. Landau [2]. We have proposed a scheme of conversion of "vertically cut" jet into energy equivalent one with another geometrical parameters.

2. Methods
2.1 Analytical solution of submerged jet
According to [2] the radial flow velocity vector component is:
\[ v_r = \frac{1}{r} F(\theta) \]  

(1)

\[ F(\theta) = 2\nu \left( \frac{A^2 - 1}{(A - \cos(\theta))^2} - 1 \right) \]  

(2)

where \( \theta \) is the angle from the jet axis, \( r \) is the radial displacement, \( \nu \) is the kinematic viscosity. Parameter \( A \) is the constant of integration determined by the radial component of the momentum flux tensor in the jet:

\[ \Pi_r = p + \rho \nu V_r \]  

(3)

where \( p \) is the pressure, \( \rho \) is the density of the liquid. For complete non-truncated jet we get the momentum flux \( W \):

\[ W = 2\pi \int_0^{\theta^*} r^2 \Pi_r \cos(\theta) \sin(\theta) d\theta \]

(4)

\[ \Pi_{r*} = \frac{4\nu^2 \rho}{r^2} \left( \frac{(A^2 - 1)^2}{(A - \cos(\theta))^4} - \frac{A}{A - \cos(\theta)} \right) \]

(5)

The equation (6) takes into account the truncate of the jet (up and down limitation by the depth of the reaction chamber \( H \)):

\[ W = \int_{\pi/2 + \theta^*}^{\pi/2 + \theta^*} r^2 \Pi_r \cos(\theta) (2\pi - 4\arcsin\sqrt{1 - (H / 2 \sin(\theta))^2}) d\theta + \int_0^{\pi/2 - \theta^*} r^2 \Pi_r \cos(\theta) \sin(\theta) 2\pi d\theta \]

(6)

Here, the boundary angle \( \theta^* \) is determined from the condition:

\[ \sin(\theta^*) = H / 2r \]

(7)

where \( H \) is the depth of the reaction chamber, \( r \) is the displacement of the loaded liquid front. The idea of an equivalent non-truncated jet is to find \( A_{corr} \) from:

\[ W'(A_{beg}) = W(A_{corr}) \]

(8)

From (1) with the zero initial condition:

\[ r = \sqrt{2F(\theta)t} \]

(9)

Therefore, if the jet parameter \( A \) and the physical characteristics \( (\rho, \nu) \) of the medium are constant, the radial displacement of the loaded liquid front is described by a simple relationship:

\[ r = \text{const} \cdot \sqrt{t} \]

(10)

2.2 Numerical study of liquid injection
The Navier-Stokes and the continuity equations were used for velocity profile simulation:
\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} \]  
\[ \nabla \cdot \mathbf{u} = 0 \]  

(11)

Simulation was carried in 3D by finite element method using COMSOL Multiphysics package [3]. Stability of the solution was checked by comparing the results with different split rank of the space and time. The results had small variations that allows us presume the small error.

3. Results and discussion

Accounting vertical cutting (6) and clarifying the radial component of the momentum flux tensor, one specifies parameter \( A \) of the equivalent jet on which its shape depends (figure 1), calculates the flow velocity which differs from the original non-truncated jet velocity and the displacement.

![Figure 1. Dependence of the projection of the radial velocity on the axis of the jet for various values of the constant \( A \).](image)

The analytical expression for the radial velocity component was calculated for the jet axis. Jet parameters were defined by the displacement during the first 0.02 seconds and were used in the analytical solution. Figure 2 (a) shows the results of simulation of the liquid front displacement during its input through 0.4 mm wide channel into a circular chamber with a diameter of 12 mm (curve (1), equation (11)) and analytical expression (the curve (2), equations (9)-(10)):

\[ 2.105 \sqrt{t} \]  

(12)

which corresponds to non-truncated jet parameters.

After the 12 seconds the curve (1) satisfies a power law with an exponent greater \( \frac{1}{2} \), which is associated with a significant effect of its cut and with a decrease in the parameter \( A \) of equivalent jet.

There is the comparison of the normalized flow velocity obtained by simulation and the normalized averaged along height radial velocity calculated analytically according to [2] in the figure 2 (b).
Figure 2(a,b). (a) Comparison of the simulation (1) of liquid sample front displacement and the analytical solutions (2); (b) Comparison of normalized velocities of liquid injection calculated numerically (●) and by submerged jet model (★) with H = 1 mm.

Approximating dependence was built for the averaged along vertical axis of jet radial velocity component. The simulation results of the liquid injection velocity into the reaction chamber with the depth of 1 mm have good qualitative and quantitative agreement with estimates obtained by the model of truncated jet. However, the averaged value of the radial velocity projection:

\[
\int_0^\pi \left( \frac{A^2 - 1}{(A - \cos(\theta))^2} - 1 \right) \cos(\theta) d\theta / \pi
\]

provides better quantitative agreement (figure 2 (b)).

Comparison of the data presented in figure 1 showed: i) displacement dependence on the time interval 0 - 9 seconds up to 6 mm has a good quality and satisfactory quantitative agreement (coefficient of determination \( R^2 = 0.992 \)); ii) the changes of radial velocity over time obtained by simulation and submerged truncated jet model (5) and (6) have shown little difference for the chamber with 1 mm depth. Discrepancy of velocities (figure 1 (b)) after 6-8 mm can be attributed to the vicinity of the chamber outer wall. In this case: a) the boundary condition is the zero normal velocity, b) velocity momentum reflects from the walls is appeared and the jet model is not correct under these circumstances.

Thus, the load of a sample through a narrow channel into the chamber can be simulated with a model of a submerged Landau jet with corrections for its vertical cut (equations (1) - (8)).

During estimation the area in which the submerged jet approximation is applicable, the important geometric parameters are chamber’s length and width.

Rectangular chambers (e. g. figure 3 (a, b)) with a widths of 12, 6, 2, 1, and 0.4 mm and depths of 200 and 1000 μm and rounded ones (e. g. figure 3 (c, d)) with the same widths (except 0.4 mm) and depths were studied by simulation (equation (11)). One of the variants of the latter is a round reaction chamber. The width of the inlet channel remained constant and equal to 0.4 mm. We considered only a part of a chamber near the sample inlet since at small Reynolds numbers (~ 1) the velocity magnitude is symmetrical with respect to an entrance and an exit of a chamber. The simulation area consisted of an input channel 0.4 mm long and a chamber with a length two times bigger than width. There was a zero pressure boundary condition at the outlet.

The dependences of the velocity along the chip axis on the distance from the input were obtained as a result of the simulation. The movement of the front was calculated from these velocities. The velocity stopped changing with increasing distance to the inlet at some distance from it as the chamber ends with a straight channel. Therefore, we were also interested in the velocity \( v_n \) normalized to its steady-state value:
\[ v_n = \frac{v_r - v_0}{v_0} \]  

(14)

where \( v_0 \) is steady-state value of velocity. Also, the width of the chamber normalized to the width of the input channel and the distance from the inlet normalized to the width of the chamber were used:

\[ D_n = \frac{D}{d} \]  

(15)

\[ r_n = \frac{r}{D} \]  

(16)

where \( D \) is the width of the chamber, \( d \) is the width of the input channel equal to 0.4 mm, \( D_n \) is the normalized width of the chamber, \( r \) is the distance from the inlet to the chamber, \( r_n \) is the normalized distance from the inlet to the chamber.

The figure 3 shows velocity distribution in different types of chambers with the widths 1 and 6 mm. Here, \( x \) and \( y \) are the coordinates counted from the beginning of the input channel. The dependences of the normalized velocities \( v_n \) on the normalized distance \( r_n \) for different chambers’ widths shown in the figure 4 (a) coincide qualitatively and quantitatively for different chambers’ depths and types.

It can be seen that the velocity almost does not change since \( r_n \) is equal to 0.5. The consequence is a transition to a uniform motion of the sample at late stages of loading. This transition tends to be linear and is more different from the submerged jet approach (10) with channel’s width decrease. This is evidenced by the approximation of dependences of displacement on time by a power function \( at^b \). Figure 4 (b) shows the dependence of \( b \) on the normalized width of the chamber \( D_n \). It was found that the index \( b \) equal 0.52 and 0.57 for the chambers’ width 12 and 6 mm, which is close to 0.5 that corresponds to a non-truncated jet according to equation (10). \( b \) increases to 0.7 when a width is 2 mm and becomes equal to 1 in the limiting case of the absence of the chamber. This is due to the fact that one of the conditions of the submerged jet model is zero velocity at an infinite distance from the inlet. A wide chamber can provide a sufficient difference between the velocity at the inlet and the steady-state velocity, while the value of \( v_0 \) begins to affect the transient process with decreasing the ratio \( D_n \). This can be seen from the decrease in the difference between the initial and final velocities and changes in the shape of the curves presented in figure 4(a).

The values of the exponents \( b \) remain fairly constant when the depth or type of the chamber changes. The approximations differ from each other mainly by the value of the coefficient \( a \).

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**Figure 3(a,b,c,d).** The distribution of liquid velocities in the horizontal cross-section along the center of the channels obtained during the simulation. (a) rectangular chamber 1 mm wide; (b) rectangular chamber 6 mm wide; (c) chamber with rounded edges 1 mm wide; (d) chamber with rounded edges 6 mm wide.
mm wide. The depth is 200 µm.

![Figure 4(a,b).](image)

**Figure 4(a,b).** (a) The dependence of the normalized velocity $v_n$ on the normalized distance $r_n$ for different widths of a rectangular chamber 200 µm deep; (b) The change of a function $a^b$ exponent obtained in approximation of the fluid front displacement with the increase of the normalized width $D_n$ of a rectangular chamber 200 µm deep.

4. Conclusions

Thus, the analytical expression based on a submerged jet approach [2] accurately describes the load of liquid sample into the reaction chamber with a ratio of its width to the width of the input channel more than 15 at a distance of half-width of the chamber from the inlet. The amendment to the jet "cut" allows to specify the dynamics of the injection during the longer time.

Acknowledgments

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