2 Mathematical Formulation

2.1 Flow models

For the study of the motion of particles different basic flows will be considered. The following first three flows are given in their analytical form. This permits to perform the validation of the code for the motion of the particle. In the second phase the discrete, numerically calculated thermocapillary flow in the half-zone is considered.

2.1.1 Analytical flows

As already mentioned, the Stuart, Taylor–Green and Arnold–Childress–Beltrami (ABC) flows can be exactly specified in every point. Furthermore, they are periodic and time-independent. This is an advantage for the mere analysis of the dynamics of the particle-flow coupling phenomenon avoiding disturbing effects due to the interpolation errors and the particle-wall or particle-free surface interaction.

Stuart vortex flow

The Stuart vortex flow consists on Stuart's one-parameter family of analytical solutions of the two-dimensional Euler equations (Stuart 1967, Pierrehumbert & Windall 1981). The general form of the stream function in dimensional units reads

$$\psi^*(x^*, y^*) = \frac{U_{\infty}L}{2\pi} \ln\left[\cosh\left(\frac{2\pi y^*}{L}\right) - \tilde{\rho}\cos\left(\frac{2\pi x^*}{L}\right)\right],\tag{2.1}$$

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which corresponds to the velocity components

$$u_x^*(x^*, y^*) = \frac{\partial \psi^*}{\partial y^*} = U_\infty \frac{\sinh\left(\frac{2\pi y^*}{L}\right)}{\left[\cosh\left(\frac{2\pi y^*}{L}\right) - \tilde{\rho}\cos\left(\frac{2\pi x^*}{L}\right)\right]},$$
(2.2a)

$$u_y^*(x^*, y^*) = -\frac{\partial \psi^*}{\partial x^*} = -U_\infty \frac{\tilde{\rho} \sin\left(\frac{2\pi x^*}{L}\right)}{\left[\cosh\left(\frac{2\pi y^*}{L}\right) - \tilde{\rho} \cos\left(\frac{2\pi x^*}{L}\right)\right]}.$$
 (2.2b)

In (2.1) and (2.2) x^* and y^* represent the dimensional position-coordinates in a cartesian frame of reference whereas u_x^* and u_y^* are the dimensional components of the velocity vector. The parameter L represents the distance between two adjacent vortices and U_{∞} the velocity of the undisturbed shear flow. The parameter $\tilde{\rho}$ is the concentration of vorticity. The value $\tilde{\rho} = 1$ indicates a periodic row of point vortices and $\tilde{\rho} = 0$ indicates a parallel shear flow. In this work the intermediate case $\tilde{\rho} = 0.25$ is considered which represents an infinite series of cat's-eye vortices along a straight line as shown in fig. 2.1. The most natural way to scale the flow results in taking the scaling parameters L_0 and U_0 , for the length and the velocity respectively, equal to L and U_{∞} , with a derived scale for the time equal to L/U_{∞} . Referring to a generic scaling velocity U_0 , so that

$$\boldsymbol{x} = \frac{\boldsymbol{x}^*}{L}, \quad \boldsymbol{u} = \frac{\boldsymbol{u}^*}{U_0},$$
 (2.3)

the resulting nondimensional velocity components read

$$u_x(x,y) = A \frac{\sinh\left(2\pi y\right)}{\left[\cosh\left(2\pi y\right) - \tilde{\rho}\cos\left(2\pi x\right)\right]},\tag{2.4a}$$

$$u_y(x,y) = -A \frac{\tilde{\rho} \sin\left(2\pi x\right)}{\left[\cosh\left(2\pi y\right) - \tilde{\rho} \cos\left(2\pi x\right)\right]},\tag{2.4b}$$

where

$$A = \frac{U_{\infty}}{U_0}.\tag{2.5}$$

This assumption permits to vary the strength of the flow A in the nondimensional equations as an independent parameter.



Figure 2.1: Stuart vortices in a $[-1, 1] \times [-0.5, 0.5]$ domain for $\tilde{\rho} = 0.25$ and A = 1. After the scaling the distance between two consecutive vortex centers is always equal to 1. The lines represent the streamlines of the flow. The arrows indicates the direction of the velocity field and the color shows the absolute value of the velocity vector.

Taylor–Green vortex flow

The Taylor–Green flow is formed by an array of counter-rotating vortices arranged in a checker-board fashion which results in rectangular convection cells (see fig. 2.2). Similar types of flow can be encountered, for example, in thermal convection with free-slip boundaries or in Langmuir circulation (Stommel 1949, Maxey 1987). The dimensional stream function is given by

$$\psi^*(x^*, y^*) = \frac{U_{max}L}{\pi} \cos\left(\frac{\pi x^*}{L}\right) \cos\left(\frac{\pi y^*}{L}\right), \qquad (2.6)$$

with the dimensional velocity components

$$u_x^*(x^*, y^*) = \frac{\partial \psi^*}{\partial y^*} = -U_{max} \cos\left(\frac{\pi x^*}{L}\right) \sin\left(\frac{\pi y^*}{L}\right), \qquad (2.7a)$$

$$u_y^*(x^*, y^*) = -\frac{\partial \psi^*}{\partial x^*} = U_{max} \sin\left(\frac{\pi x^*}{L}\right) \cos\left(\frac{\pi y^*}{L}\right), \qquad (2.7b)$$

where U_{max} represents the velocity maximum. Following the scaling presented in



- Figure 2.2: Taylor–Green vortices in a $[-1,1] \times [-1,1]$ domain for A = 1. After the scaling the distance between two consecutive vortex centers is always equal to 1. The lines represent the streamlines of the flow. The arrows indicates the direction of the velocity field and the color the absolute value of the velocity vector.
- (2.3) the nondimensional form of the velocity components reads

$$u_x(x,y) = -A\cos\left(\pi x\right)\sin\left(\pi y\right),\tag{2.8a}$$

$$u_y(x,y) = A\sin\left(\pi x\right)\cos\left(\pi y\right),\tag{2.8b}$$

with

$$A = \frac{U_{max}}{U_0}.$$
 (2.9)

Arnold–Beltrami–Childress vortex flow

The Arnold–Beltrami–Childress flow, usually known under the acronym ABC flow, is a three-dimensional periodic flow (see fig. 2.3). It is an inviscid flow and it is the solution of the three-dimensional Euler equation. The dimensional form of the velocity components reads

$$u_x^*(x^*, y^*) = U_A \sin\left(\frac{\pi z^*}{L}\right) + U_B \cos\left(\frac{\pi y^*}{L}\right), \qquad (2.10a)$$

$$u_y^*(x^*, y^*) = U_B \sin\left(\frac{\pi x^*}{L}\right) + U_A \cos\left(\frac{\pi z^*}{L}\right), \qquad (2.10b)$$

$$u_z^*(x^*, y^*) = U_C \sin\left(\frac{\pi y^*}{L}\right) + U_B \cos\left(\frac{\pi x^*}{L}\right).$$
(2.10c)

The dimensional parameters U_A , U_B and U_C represent the strength of the flow. Taking the generic velocity U_0 as scaling factor it results

$$A = \frac{U_A}{U_0},\tag{2.11a}$$

$$B = \frac{U_B}{U_0},\tag{2.11b}$$

$$C = \frac{U_C}{U_0},\tag{2.11c}$$

and the scaled flow takes the form

$$u_x(x,y) = A\sin(\pi z) + C\cos(\pi y),$$
 (2.12a)

$$u_y(x,y) = B\sin(\pi x) + A\cos(\pi z),$$
 (2.12b)

$$u_z(x,y) = C\sin(\pi y) + B\cos(\pi x).$$
 (2.12c)

2.1.2 Flow in the half-zone

The half-zone model of the floating-zone process consists of a cylindrical volume of liquid confined between two differentially heated circular rods of radius R at a distance d, and a free lateral surface. The rods are kept at constant different temperatures $T_0 + \Delta T/2$ and $T_0 - \Delta T/2$ (fig. 2.4), where T_0 is the mean value of the temperature. On the free cylindrical surface temperature-induced surface-tension gradients drive an axisymmetric steady toroidal vortex flow. In the range of large Prandtl numbers (Pr > 1), above a critical Reynolds number Re_c the flow becomes three-dimensional and oscillatory. The critical Reynolds number is proportional to the critical temperature difference ΔT_c . In the supercritical case (Re > Re_c) a pair of counter-rotating traveling waves in azimuthal direction arises. This is an unstable state and one of the two traveling wave decays leaving only one wave propagating azimuthally. In fig. 2.5



Figure 2.3: Arnold-Beltrami-Childress flow with A = B = C = 1 plotted over a three-dimensional spatial period $[-1, 1] \times [-1, 1] \times [-1, 1]$. The color represents the absolute value of the velocity vector: toward the red the strongest velocities and toward the blue the stagnation points. The black lines represent the streamlines of the flow.