CFD Modelling of a Spray Deposition Process of Paint

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Summary: The paint deposition process by spraying has been studied by means of Computational Fluid Dynamics in order to predict the final thickness of the coating and to determine theoretically the overspraying phenomenon. The VOF model has been used to describe the impact phenomena onto the wall and the Euler-Lagrange approach to simulate droplet trajectories on their way to the surface.
Particular attention has been devoted to the prediction of the maximum diameter reached by an impinging droplet at the end of the spreading phase. This diameter is very important in the study of the paint processes because the high viscosity and the small surface tension of paints reduce the impingement practically only to the spreading phase. Two different configurations of atomizers have been considered. The air flux provides a finer atomisation of the liquid, gives to the droplets the necessary velocity to reach the wall, but is also the main cause of overspray since the small droplets tend to follow its deviation near the wall.

Key words: CFD, simulation, drop impact , spray, spread

Introduction

Sprays are widely used in many applications as the pouring out of herbicides in agricultural field, the injection of fuel in combustion engines or the deposition of paint in coating processes. In all these processes, a detailed knowledge of the behaviour of droplets, from the outlet of the atomizer to the target surface, is very useful in order to achieve either uniform deposition, or good combustion or the desired aspect of the coating. To characterise the whole process after its atomisation, the aerodynamic transport of the droplets and the collision onto the surface are treated separately. The distinction allows us to study more deeply the phenomenon of impact, helping to better understand what happens near the surface to cover. The power growth of diesel engines achieved in recent years or the saving of paint in industrial application are two example of the usefulness of these studies.

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The outcome of the impingement of a single droplet may be its deposition on the surface or its reatomization into smaller secondary droplets with partial mass deposition. The result of the impingement is determinated by the properties of the fluid such as viscosity and surface tension as well as by the diameter of the droplet and its velocity relative to the wall. Furthermore, the surface roughness, the thickness of the liquid film and the wall temperature are important. Previous investigations [1-5] revealed that the droplets spread out on the surface and form a liquid film only if the component of moment normal to the wall is small; otherwise they form a conical sheet similar to a crown, that may disintegrate into secondary droplets.

When a droplet spreads onto a surface forms a thin liquid disk that is usually called *lamella*. First, the lamella expands very quickly and reaches a maximum radius within a short time. The kinetic and surface energy of the drop are dissipated by viscous processes in the thin sheet of liquid, and are transformed in additional surface energy. During a second stage the lamella shrinks to a small size, and in some case the recoil of the lamella may cause the drop to separate from the surface and rebound.

The thickness of the liquid and the final radius of the lamella depend above all on the viscosity of the liquid and on interfacial tensions between both liquid and gas and liquid and surface. One can calculate the dimensions of the lamella by tracking the interface between liquid and air by mean of the VOF model [6,7]. In this model a single set of momentum equations is shared by the fluids, and the volume fraction of each fluid is tracked throughout the domain. The VOF model can also include the effects of surface tension and contact angle.

To simulate a spray deposition process it is also important to know how many droplet reach the wall and where they impact. In order to achieve this aim, the droplet trajectories have been calculated by mean of the Euler-Lagrange approach. [8]

Modelling of the impact zone

If thermal effects are negligible, a dimensional analysis indicates that the impact can be described in terms of the following dimensionless parameters: [5,9]

1. Reynolds number, $\mathrm{Re}=\dfrac{\rho D V}{\mu}$
2. Weber number, $\mathrm{We}=\dfrac{\rho D V^2}{\sigma}$
3. Dimensionless surface roughness, $R_s^*=2R_s/D$

4. Dimensionless film thickness, $F_l^*=F_l/D$

5. Bond Number. $\mathrm{Bo}=\dfrac{\rho D^2 g}{\sigma}$

Another number often used in literature is Ohnesorge number, defined as:

$$\mathrm{Oh}=\frac{\mu}{\sqrt{\rho D\sigma}}=\frac{\mathrm{We}^{1/2}}{\mathrm{Re}}$$

In our case Bo and F_l can be neglected, since we have considered small droplets with low impact velocity colliding dry surfaces. The dynamic of spreading is characterized primarily by We and Re numbers (or Oh), by roughness and finally by the contact angle.

When a droplet impacts onto a surface it normally forms a thin liquid disk that is called *lamella*, which expands quickly and reaches a maximum diameter d_m: this phenomenon is called spread. Subsequently shrinks due to surface tension, and in some cases, when the elastic force is very strong in comparison to viscous dissipation, some tiny droplets are formed from the centre of the lamella. Normally after the recoiling phase, a new spread can be observed followed by a new retraction and so on till the liquid has reached its equilibrium shape [10]. The thickness of the liquid and the final radius of the lamella depend mainly on the viscosity of the liquid and interfacial tensions between liquid and gas and liquid and surface. A parameter of great interest in coating process is the maximum diameter d_m reached by the lamella after its spread. Many authors [1-3,11], have considered that the total energy owned by the drop before impact is equal to that of the lamella at its maximum diameter minus the energy dissipated by friction:

$$\underbrace{E_k + E_p + E_s}_{\text{Before impact}} = \underbrace{E_k + E_p + E_s}_{\text{After impact}} + E_{diss} \tag{1}$$

where subscripts k, p, s and *diss.* refer to kinetic, potential, surface and dissipated energy, respectively. Coupling this balance with simplified models of the spreading phase, some authors have developed simple equations for the maximum spreading ratio, that is: $B_m = d_m/D$ (D being the size of the droplet before impact. An example of this equation proposed by Moo *et al.* [12]:

$$\left[\frac{1}{4}(1-\cos\theta)+0.35\frac{\mathrm{We}}{\sqrt{\mathrm{Re}}}\right](B_m)^3-\left(\frac{\mathrm{We}}{12}+1\right)(B_m)+\frac{2}{3}=0 \tag{2}$$

Another one, that is Chandra and Avedisian [2]:

$$\frac{2\,\mathrm{We}}{3\,\mathrm{Re}}(B_m)^4 + (1-\cos\theta)(B_m)^2 - \left(\frac{\mathrm{We}}{3}+4\right) = 0 \tag{3}$$

In order to predict the time evolution of the size of the lamella, some expressions like $B(\tau)=h[1\text{-}\exp(-k\tau)]$, where τ is a non dimensioned time, have been proposed. One of these is: [9]

$$B(\tau) = 2.4[1-\exp(-0.9\tau)] \qquad \text{with} \qquad \tau = t\sqrt{\frac{\sigma}{\rho R^3}}, \tag{4}$$

Scheller and Bousfield [13] have connected a large number of experimental data according to the relationship:

$$B_m = 0{,}61\left(\mathrm{Re}^2\,\mathrm{Oh}\right)^{0{,}166} \tag{5}$$

The range of considered Re is from 19 to 16400, while We is between 0.002 and 0.58.

In some cases the outcome of the impact of a droplet on a surface may be its reatomization into smaller secondary droplets with partial mass deposition, and not its spreading. Such a phenomenon is called "splashing". Previous investigations [1,4-5] revealed that the droplets spread out on the surface and form a liquid film only if the component of moment normal to the wall is small; otherwise they form a conical sheet similar to a crown, that may disintegrate into secondary droplets. When a single droplet hits a surface, the non-dimensional parameter K determines whether it is completely deposited or partially splashed into secondary droplets. The parameter K can be calculated from correlations like $K=Oh\ Re_l^a$, where a is a constant. According to Mundo *et al.* [5], a assumes the value of 1.25, whereas for Yarin and Weiss [4], it has the value of 1.27. If K is smaller than a critical value K_{crit}, depending on the surface condition, the droplet is completely deposited and forms a liquid film on the surface. If K exceeds the critical value, a crown structure is formed around the point of impingement. The value of K_{crit} is higher for dry and smooth surfaces. The influence of surface roughness can be taken into account with the non-dimensional surface roughness number R_s^*. For low values of R_s^* K_{crit} is very high, as the out flowing fluid at the contact line between the impinging droplet and the surface cannot be redirected in a direction normal to the wall. Rising the surface roughness, K_{crit} decreases strongly at first and reach an asymptotic value for high non-dimensional roughness numbers [14]. For coating sprays, K should be small as possible in order to spread all the paint that arrives onto the surface. For this reason, droplets have small sizes and the paint is extremely viscous.

Results

Simulation of the impact of single droplets upon dry and smooth surface have been done concerning droplet different in size and velocity. The drop diameter has been varied from 25 to 200 μm, whereas the drop velocity from 5 m/s to 20 m/s. The CDF code Fluent has been used in its version 5.0 with the VOF model. Neglecting the possible instability at the rim of the lamella, axis symmetric conditions can be imposed and a 2D grid developed. The grid has been made of square cells with the edge from 1.5 μm to 2μm, depending of the droplet size. The simulations have been carried out with a constant time step equal to 10^{-9} s. This step assures a quite fast convergence from the beginning to the end of the simulation and it is proportionate to the length scale of the case. Some 3D simulation are also been performed. Regarding the characteristic of the liquid, we have considered a new paint without any organic solvent: for the viscosity we have adopted a value of 40 cP while for the surface tension a value equal to 0.03 N/m has been used. The contact angle has normally been kept constant at a value of 70°, corresponding to the advancing angle. This simplification should not lead to significant error since, in the considered case, the recoiling phase is negligible (as verified adopting a dynamic contact angle). An additional consequence is that the final size of the lamella is very close the largest diameter by the lamella after spreading. The behaviour is due to the high viscosity (40 cP) which dissipate all the inertia of the droplet and to the small surface tension which is not able to give enough elastic energy to retract the lamella. The sequence of Figure1. confirms such a behaviour.

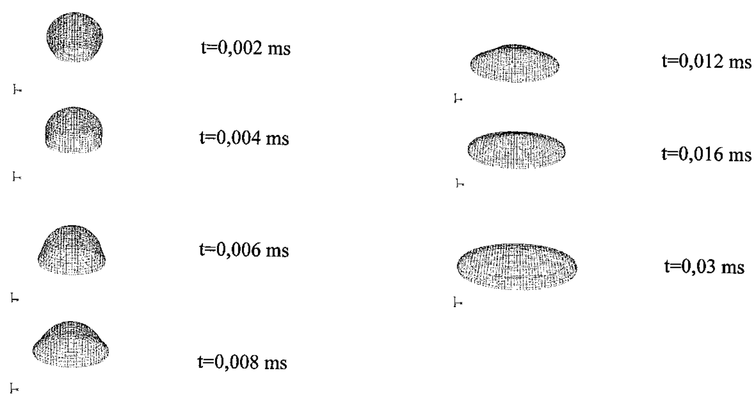

Figure 1. Impact of a 200 μm diameter paint droplet at 5 m/s colliding a smooth surface.

The figure represents the impact of a droplet of 200 μm of diameter colliding at 5 m/s. Another important aspect for the considered paint deposition process is that we have never observed any slashing. That has been also confirmed by parameter $K = \mathrm{We}^{0,5}\,\mathrm{Re}^{0,25}$, which is always smaller than its critic values found for smooth surfaces [5]. Figure 2. (a) reports the values of the maximum spread factor calculated by CFD as a function of Re at different Ohnesorge numbers.

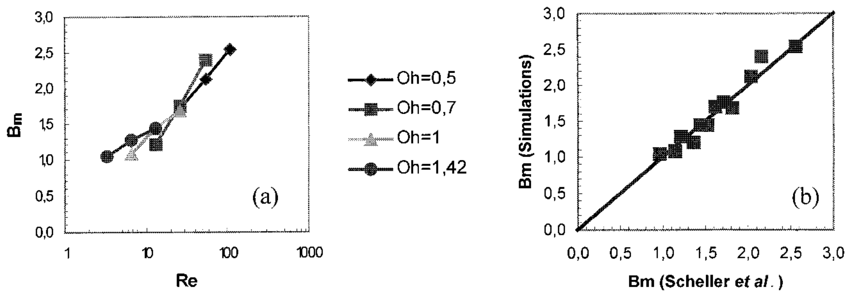

Figure 2. (a) Maximum spread predicted with CFD simulations as a function of Re at different Oh. (b) Comparison of the maximum spread obtained with CFD simulation to that predicted with the Scheller correlation.

Obviously increasing the impact velocity a larger lamella is obtained due to the greater inertia that must be dissipated. In Fig. 2. (b) are compared the results found by the simulations with the predictions of the correlation of Sheller [13]. The figure shows a good agreement between our results and the experimental study, although the range where it has been done does not cover all our tests.

Modelling of spraying phase

The prediction of the fluid flow of the continuous phase was obtained by solving the time-averaged Navier-Stokes equation in connection with a closure model for turbulence [15]. The equations of motion for a steady flow in turbulent regime, expressing the instantaneous values of the quantities by Reynolds decomposition, can be written in the following way:

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{6}$$

$$\rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \mu \frac{\partial^2 U_i}{\partial x_j^2} - \rho \frac{\partial}{\partial x_j}(\overline{u_i' u_j'}) + S_{p,\phi} \tag{7}$$

where U_i is the average velocity component along axis x_i and u_i is the fluctuating velocity along the same axis. The solution of this equation requires the knowledge of a relationship (closure equation) between the mean velocity field and the Reynolds tensor (the term composed by the fluctuating velocities). The Reynolds tensor can be expressed as a function of the rate of strain tensor S_{ij} as follows:

$$-\rho(\overline{u_j^{'} u_i^{'}}) = 2\mu_t S_{ij} \tag{8}$$

where μ_t is the turbulent viscosity and in the k-ε model is calculated as:

$$\mu_t = C_\mu \rho \frac{k^3}{\varepsilon} \tag{9}$$

where k is the kinetic energy of the fluctuating flow, ε the turbulent dissipation rate and C_μ is constant.Of course, two equations that describe the variation of the turbulent kinetic energy k and of the turbulent dissipation rate ε are needed. They can be expressed as:

$$U_i \frac{\partial k}{\partial x_i} = -\frac{1}{\rho}\frac{\partial}{\partial x_i}\left(-\Gamma_k \frac{\partial k}{\partial x_i}\right) + \frac{2\mu_t}{\rho} S_{ij} S_{ij} - \varepsilon \tag{10}$$

$$U_i \frac{\partial \varepsilon}{\partial x_i} = \frac{1}{\rho}\frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_i}\right) + \frac{2\mu_t}{\rho} C_{\varepsilon 1} S_{ij} S_{ij} - C_{\varepsilon 2}\frac{\varepsilon}{k} \tag{11}$$

The empirical constants of the turbulence model are: $C_\mu = 0.09$; $C_{\varepsilon 1} = 1.44$; $C_{\varepsilon 2} = 1.92$. The additional source terms $S_{p,\phi}$ are introduced to account for the influence of droplets on the fluid flow. Detailed equations, which describe these source terms, are available in the article by Ruger *et al* [16]. The dispersed phase is treated by the Lagrangian approach, where a large number of droplet parcels, representing a number of real droplets with the same properties, are traced through the flow field. The representation of droplets by parcels makes it possible to consider size distribution and to simulate the measured liquid mass flow rate at the injection locations by a reasonable number of computational droplets. The trajectory of each droplet parcel is calculated solving the equation of motion for a single droplet. The basic equation of motion is the result of the force balance on the particle written in a Lagrangian reference frame. A basic equation of motion can be written neglecting the forces due to pressure gradients, virtual mass and history terms. This equation of motion has the following form, for the x direction in Cartesian co-ordinates:

$$\frac{dU_{p,i}}{dt} = F_D\left(U_i - U_{p,i}\right) + g_i \frac{\left(\rho_p - \rho\right)}{\rho_p} + F_i \tag{12}$$

Where $F_D(U_i - U_{p,i})$ is the drag force per unit particle mass and

$$F_D = \frac{18\mu}{\rho_p D_p^2} \frac{C_D \mathrm{Re}}{24} \tag{13}$$

Here, U is the fluid phase velocity, U_p is the particle velocity, μ is the molecular viscosity of the fluid, ρ is the fluid density, ρ_p is the density of the particle and D_p is the particle diameter. Where Re is the relative Reynolds number, which is defined as

$$\mathrm{Re} = \frac{\rho D_p \left| \left(\overrightarrow{U_p} - \vec{U} \right) \right|}{\mu}. \tag{14}$$

The drag coefficient C_D has been calculated from the following equation [17]:

$$C_D = \frac{24}{\mathrm{Re}} \left(1 + 0.15 \mathrm{Re}_p^{0.687} \right) \qquad Re_p < 500 \tag{15}$$

In order to model the droplet dispersion in turbulent flow and to obtain a representation of the local velocity, the so-called eddy lifetime concept can be applied [18]. This model assumes that the droplet interacts with a sequence of turbulent eddied with randomly sampled fluctuations.

Results

Hereafter the results of the simulation of two different types of sprays normally used in coating process are reported. The droplet trajectories have been determined with the Euler-Lagrange approach implemented in Fluent. Inlet boundary conditions have been specified inside the gun for the air phase in order to achieve a better representation of turbulence at the nozzle, whereas for the paint, its mass flux, the distribution of the droplets and their inlet velocity has been prescribed immediately after the exit of the gun.

The air flow rate is one of most interesting parameters since it influences the formation of droplets, increases the impact velocity and plays an important role on the overspray phenomena. In Figures 3 and 4, the simulated air velocity vectors and the droplet trajectories for a low volume middle pressure gun are reported.

This type of gun normally operates with an air cup pressure of 0.20 MPa, consumes 300 Nl/min of air, 300 cc/min of paint with an efficiency of about 70 %. The diameter of the nozzle is 2 mm and the thickness of the circular section for the air 1.5 mm. The distance from the wall is of 20 cm and a Rosin-Rammler droplet size distribution has been used with a mean diameter of 36 μm and a spread factor of 2.11.

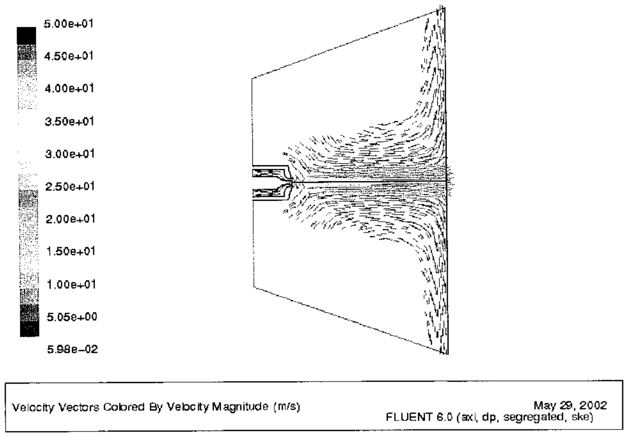

Figure 3. Velocity vectors contoured by velocity magnitude of a paint spray referring to a low volume middle pressure gun.

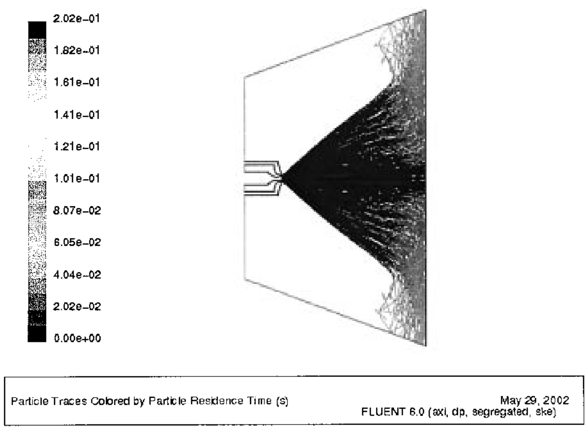

Figure 4. Particle tracks contoured by particle residence time referring to a low volume middle pressure gun.

The CFD simulation predicts a value of efficiency of about 65%, close to that given by the manufacturer. Looking at the particle tracks it appears that many droplets are deviated by the air stream and exit from the computational domain, confirming that the loss of paint is due essentially to the deviation of droplets by the air and not to splashing phenomena.

The other type of gun considered is a standard one. It differs from the previous configuration in air consumption (500 Nl/min) and cup pressure (0.35 MPa). The simulation shows the formation of a narrower cone and, even if the distance between the nozzle and the wall is now of 25 cm, it is still evident the droplet deviation. For this gun a smaller efficiency, has been found, of about 45 %. In agreement with the data of the manufactured, this could be explained with the larger air amount that forms an air pillow onto the wall, but it could also be due to the different inlet pressure of the liquid paint.

Conclusions

In this paper, a possible approach for the simulation of a coating process by spraying, using a commercial CFD code has been described. In order to characterize what happens at the wall, the impacts of a single droplet has been studied with the VOF model. The simulations have shown that all the liquid of the droplet remains on the wall during the wall impact and that a possible splash or rebound is avoided due to the high viscosity and the small surface tension of the paint.

Furthermore the friction caused by the high viscosity of the liquid dissipates all the inertia of the droplet and stops practically the impact when the lamella of liquid has reached its maximum diameter. The maximum spread and the thickness of the liquid film has been valuated.

In order to know the paint flux on the target surface, the droplet trajectories have been calculated with the Euler-Lagrange approach. Two types of spraying guns normally used in the coating industry have been considered and the effect of the air flux onto the droplet has taken into account. Since air is the main cause of the waste of paint, the overspray factor has been determined.

References

[1] M. Rein, "Phenomena of liquid drop impact on solid and liquid surfaces", *Fluid Dyn. Res.*, **1993**, *12*, 61.

[2] S. Chandra, C. T. Avedisian, "On the collision of a droplet with a solid surface", *Proc. R. Soc. London*, **1991**, *432*, 13.

[3] C. D. Stow, M. G. Hadfield, "An experimental investigation of fluid flow resulting from the impact of a water drop with an unyielding dry surface", *Proc. R. Soc. London*, **1981**, *373*, 419.

[4] A. L. Yarin and D. Weiss, "Impact of drops on solid surfaces: Self-similar capillary Waves, and splashing as a new type of kinematic discontinuity", *J. Fluid Mech.*, **1995**, *283*, 141.

[5] C. Mundo, M. Sommerfeld, C. Tropea, "On the modeling of liquid sprays impinging on surfaces", *Atomization and Sprays*, **1998**, *8*, 625.

[6] D. B. Kothe, R. C. Mjolsness and M. D. Torrey, "A computer program for incompressible flows with free surfaces", *Technical Report*, **1991**, *LA-12007-MS, LANL.*

[7] C. W. Hirt, B. D. Nichols, "Volume of fluid (VOF) method for the dynamics of free boundaries", *J. Comput. Phys.*, **1981**, *39*, 201.

[8] M. Ruger, S. Hohmann, M. Sommerfeld and G. Kohnen, "Euler/Lagrange calculations of turbulent sprays: the effect of droplet collisions and coalescence", *Atomisation and Sprays*, **2000**, *10*, 47.

[9] S. Schiaffino, A. A. Sonin, "Molten drop deposition and solidification at low Weber numbers", *Phys. Fluids*, **1997**, *9*, 3172.

[10] R. E. Ford and C. G. L. Furmidge, "Impact and spreading of spray drops on foliar surfaces Wetting", *Soc. Chem. Ind.*, **1967**, *25*, 417.

[11] G. Trapaga and j. Szekely, "Mathematical modeling of the isothermal impingement o liquid droplets in spraying processes", *Metall. Trans.*, **1991**, *B22B*, 901.

[12] T. Mao, D. C. S. Kuhn, H. Tran, "Spread and rebound of liquid droplets upon impact on flat surfaces", *AIChE J.*, **1997,** *43*, 2169.

[13] B. L. Scheller, D. W. Bousfield, "Newtonian drop impact with a solid surface", *AIChE J.*, **1995**, *41*, 1357.

[14] M. Bussmann, J. Mostaghimi, S. Chandra, "Modeling the splash of a droplet impacting a solid surface", *Phys. Fluids,* **2000**, *12*, 3121.

[15] B. E. Launder and D.B. Spalding, "The numerical computation of turbulent flows", *J. Comput. Meth. Appl. Mech. Eng.*, **1974**, *3*, 269.

[16] M. Ruger, S. Hohmann, M. Sommerfeld and G. Kohnen, "Euler/Lagrange calculations of turbulent sprays: the effect of droplet collisions and coalescence", *Atomization and Sprays*, **2000,** *10*, 47.

[17] B. J. Daly and F. H. Harlow, "Transport equations in turbulence", *Phys. Fluids*, **1970**, *13*, 2634.

[18] R. Clift and W.H. Gauvin, "The motion of particle in turbulent gas stream", *Chemeca,* **1970**, *70*, 14.