Numerical Investigation on Modeling of Flue gas Condensation by using Multiphase and Multispecies Approach in CFD

Ugraram Raghavendra
Department of Mechanical engineering, Intell Engineering College, Anatapur 515004, India.

Abstract

In this paper, a numerical study is carried out by using an approach of multiphase multi species modeling on condensation of water vapor from a mixture of flue gas in Boiler pipe. Due to the surface temperature less than the dew point of the vapor-gas mixture, the Condensation occurs .The main focus of this study is to capture the thin film of water formed due to the effect of heat transfer and pipe bend. Also the effect of mass flow rate of flue gas on volume fraction of water vapor formed is also studied. Results from the study evaluates capability of computational fluid dynamics (CFD) Ansys solver FLUENT to capture the physics of condensation, for two different phases of fluid with its species and it predicts the formation of water film and volume fraction, thus these results can be used in the design and optimization of flue gas pipe in Boilers.

KEYWORDS: Condensation, Numerical study, Flue gas, CFD

1. Introduction:

Figure 1.1 shows the Geometry of Boiler pipe in which the flue gas is cooled by Air. The principle of flue gas cooling is analogous to concentric tube reverse flow heat exchanger. The phenomenon of local condensation depends on the flow rate of flue gas, air and the fluid flow due to the pipe geometry.

Flue gas is considered as combination of species of CO2, Nitrogen & water vapor and is assumed that there is no non-condensable gas present in flue gas. The heat transfer between Flue gas & air happens through the aluminum pipe which is of 2mm thickness.

When water vapor content in flue gas is in contact with solid surface and if the surface temperature is less than the saturation temperature of vapor, then the condensation occurs. Thus condensed water forms a liquid film, which is attached to the walls and propagates along the flow. Along the flow direction the thickness of the liquid film amplifies as more and more vapor gets in contact with the solid walls. Eventually this liquid film forms an interface between flue gas and solid walls & resists against heat transfer. Further down the flow direction the heat released due to vapor condensation should transmit though the liquid film before it comes within reach of the cooling solid surface.

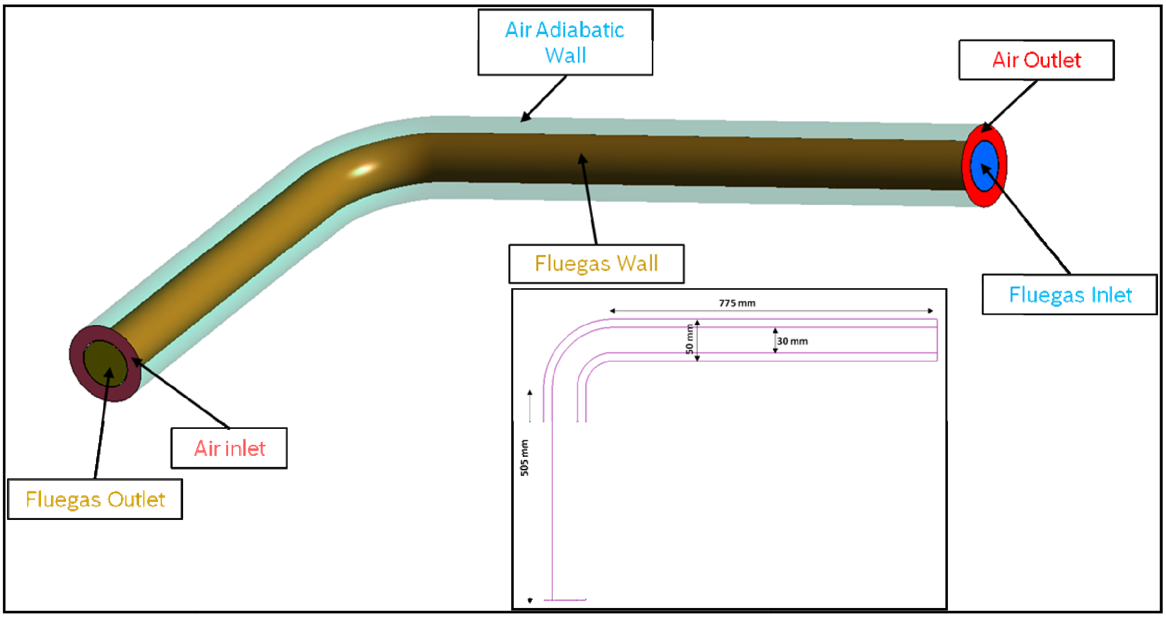

Figure 1.1 Geometry of Boiler Pipe

2. Numerical approach:

2.1 Governing Equations

CFD is based on the fundamental governing equations of fluid dynamics (Continuity, momentum, and energy equations). Governing equations are mathematical statements of the physical fundamental principle. The physical aspects of any fluid flow are governed by the following fundamental principles.

a) Conservation of mass

b) Conservation of momentum (Newton's second law)

c) Conservation of energy (first law of thermodynamics)

The governing equations for a three-dimensional, compressible, viscous flow are:

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho v) = 0$$

Where $$\nabla = \frac{\partial}{\partial \mathrm{xi}}\mathrm{i} + \frac{\partial}{\partial \mathrm{xj}}\mathrm{j} + \frac{\partial}{\partial \mathrm{xk}}\mathrm{k}$$

$$v = u_i i + u_j j + u_i k$$

Momentum equation:

$$\rho \frac{DV}{Dt} = \nabla.\tau ij - \nabla p + \rho F$$

Energy equation:

$$\rho \frac{De}{Dt} + p(\nabla.V) = \frac{\partial Q}{\partial t} - \nabla.q + \emptyset$$

Where □ is the fluid density, V is the fluid velocity vector, $\square_{ij}$ is the viscous stress tensor, p is pressure, F is the body forces, e is the internal energy, Q is the heat source term, t is time, ∅ is the dissipation term.

Depending on the nature of physics governing the fluid motion, one or more terms might be negligible. These fundamental principles can be expressed in terms of mathematical equations, which will in their most general forms such as partial differential equations. CFD is the art of replacing the governing partial differential equations of fluid flow with numbers and advancing these numbers in space and / or time domain to obtain a final description of complete flow field of interest. With the development of high-speed digital computers, CFD has become a powerful tool to predict flow characteristics in varied problem, in an economical way.

Species Transport Equations:

When you choose to solve conservation equations for chemical species, ANSYS FLUENT predicts the local mass fraction of each species, Y_i, through the solution of a convection-diffusion equation for the i_{th} species. This conservation equation takes the following general form:

$$\frac{\partial}{\partial t}(\rho Yi) + \nabla.(\rho \vec{v} Yi) = -\nabla.\vec{Ji} + Ri + Si$$

Where R_i is the net rate of production of species i by chemical reaction and S_i is the rate of creation by addition from the dispersed phase plus any user-defined sources.

2.2 Simulation Model

To perform a multiphase multi species steady state CFD simulation, a 3D model of above discussed geometry is modeled in FLUENT to capture condensation of Flue gas. The main objective of the simulation is to compute

- ✓ Amount of water condensation in the flue gas
- ✓ Temperature distribution of flue gas
- ✓ Evolution of flue gas species fraction

2.3 Mesh details:

- ✓ Element type : Hex
- ✓ Number of Nodes : 0.81 Million

Number of Elements : 0.74 Million

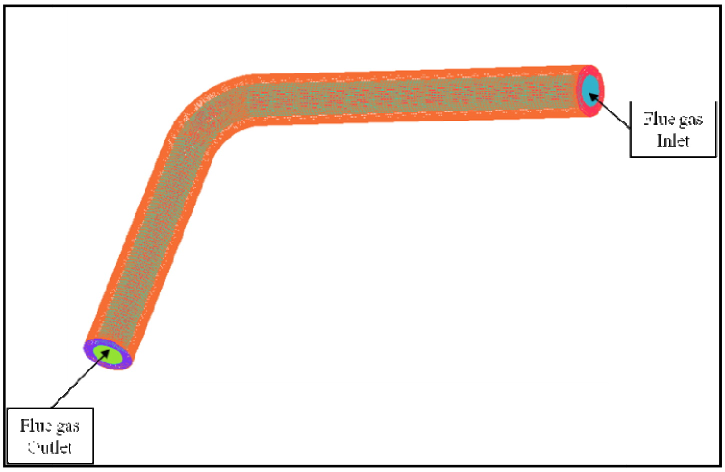

Figure: 2.1 Mesh details

2.4 Solver details:

- ✓ Solver : 3D, Pressure based solver
- ✓ Phase change model : Evaporation-Condensation model
- ✓ Time marching : Steady state
- ✓ Numerical Discretization : High resolution
- ✓ Mathematical model : Flow ,turbulence, phase, species and energy
- ✓ Turbulence model : SST scheme

2.5 Case studies:

The investigation is carried out with two main cases. In these cases the effect of mass flow rate of flue gas on condensation behavior is studied. Two Mass flow rates of Flue gas are considered and the variation in water film formation, volume fraction of water & temperature of flue gas are computed. In case 1 the flue gas mass flow rate is 0.0206 kg s^{-1} and in case 2 the mass flow rate is reduced by 100 times (i.e. 0.000206 kg s^{-1}).

2.6 Boundary conditions:

Case 1:

Boundary conditions		**Air**	**Flue gas**
Inlet	Flow rate [kg s^{-1}]	0.01936	**0.0206**
	Temperature [K]	300	400
	$h_2$0 Mass fraction [%]	--	15.85
Outlet	Pressure Outlet [bar]	0	0

Case 2:

Boundary conditions		**Air**	**Flue gas**
Inlet	Flow rate [kg s^{-1}]	0.01936	**0.000206**
	Temperature [K]	300	400

	$h_2 0$ Mass fraction [%]	--	15.85
Outlet	Pressure Outlet [bar]	0	0

3. Results and Discussion:

Modeling of condensation with multiphase and multi species in FLUENT started with many trail cases, where initially cooling of flue gas with its corresponding species is only modeled. The accuracy of results is evaluated by several checks.

As a second trail air, solid & flue gas domains are modeled with air as the primary phase and flue gas as secondary phase with its species and observed that the contour plots of temperature, volume fraction of water satisfy the boundary conditions. Grid independent study is carried out and concluded that the results are independent of grid size.

Contours of temperature, water liquid volume fraction and mass fraction of $h_2 o$ species of flue gas are plotted in mid plane.

Results Case 1:

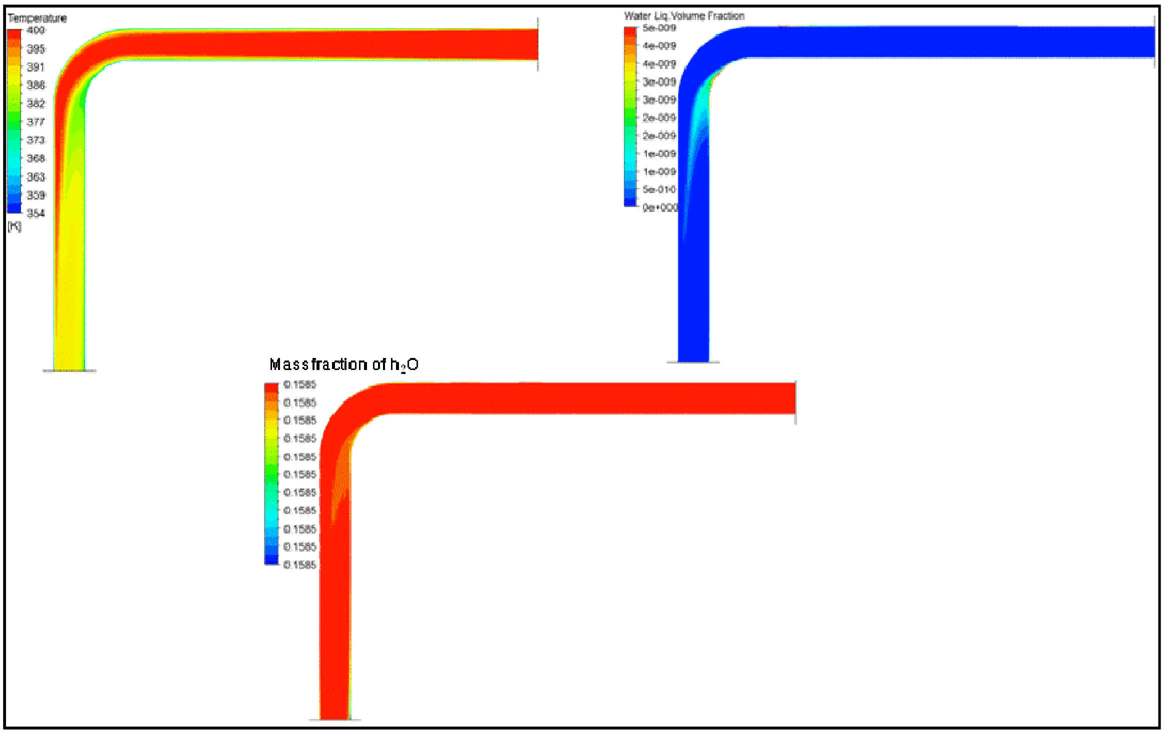

Figure: 3.1 Case 1 flue gas Contours

Results Case 2:

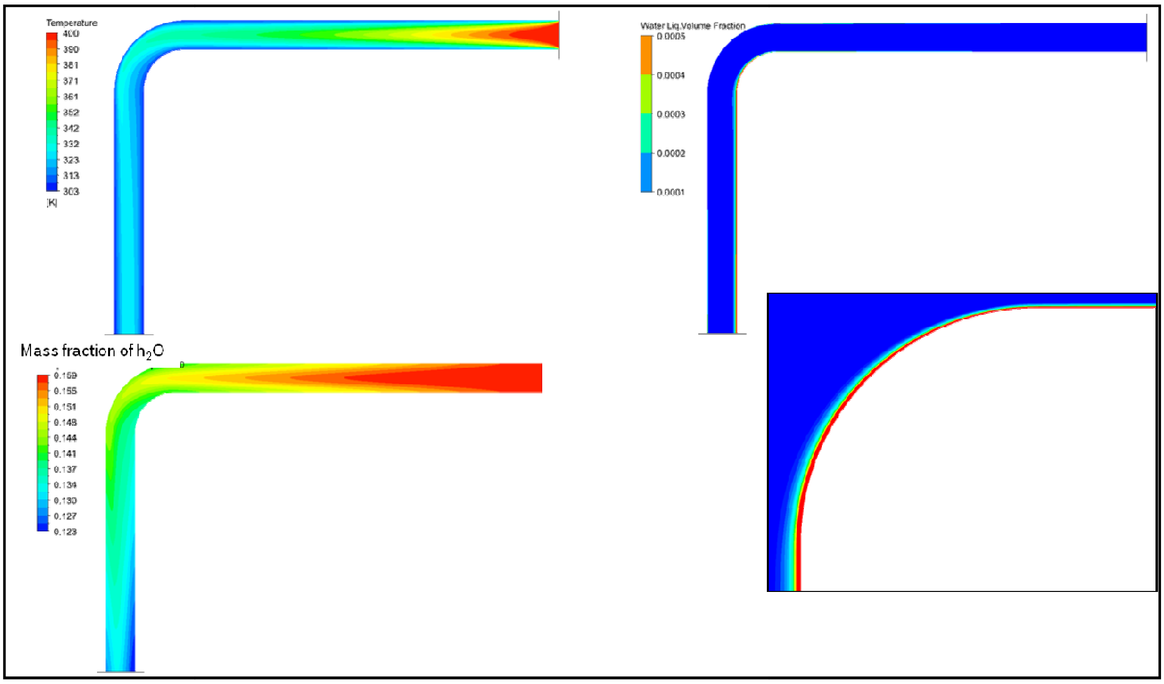

Figure: 3.2 Case 2 flue gas Contours

From the results, it is observed that the formation of liquid film is more sensitive to inlet mass flow rate of flue gas. Lower inlet mass flow rate of flue gas promotes more formation of liquid film. The thickness of the liquid film tends to grow at a faster rate when the flow passes the 90 degree bend.

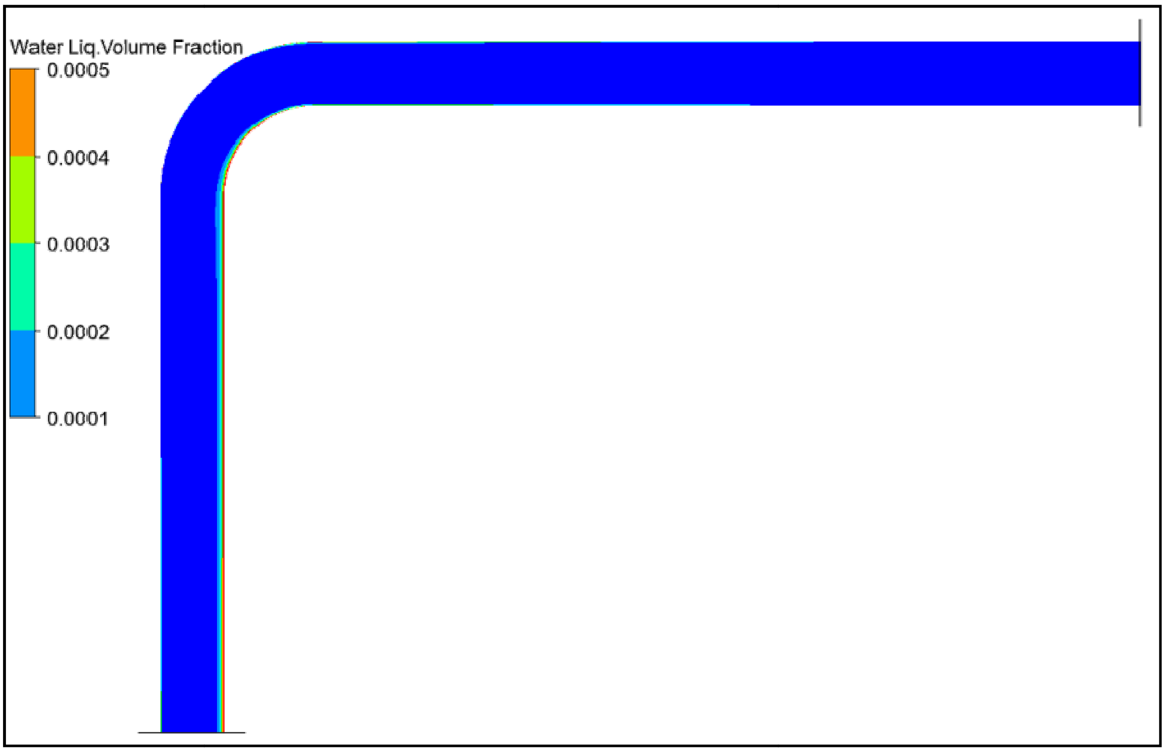

Figure: 3.3 Case 2 Water liquid volume fraction in flue gas contour

The table below consolidates and compares the quantitative values of outputs of Case 1 & Case 2.

Parameter	Case 1	Case 2
Volume fraction of Water-liquid in Flue gas domain (Volume Average)	3.30E-10	0.00078
Mass fraction of Water-vapor in Flue gas domain (Volume Average)	0.1585	0.145
Drop in Temperature of Flue gas [K]	11.65	81.212
Rise in Temperature of Air [K]	15.15	2

4. Conclusions:

Simulation results of flue gas condensation with Multiphase multispecies simulation for two different mass flow rate conditions of flue gas are presented. The main objective of computing water vapor condensation and water film formation with its volume fraction is achieved.

4.1 Summary:

- ✓ Simulation set up in Ansys FLUENT to capture water vapor condensation is capable of predicting the water film formation.
- ✓ Volume fraction of condensed water increases with decrease in inlet flow rate of flue gas.
- ✓ 90 degree pipe bend shows a significant influence on thickness of water film.

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