

Implementation and validation of the condensation model for containment hydrogen distribution studies



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HIGHLIGHTS

- A condensation model based on diffusion was implemented in FLUENT.
- Validation of a condensation model for the H₂ distribution studies was performed.
- Multi-component diffusion is used in the present work.
- Appropriate grid and turbulence model were identified.

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ABSTRACT

This paper aims at the implementation details of a condensation model in the CFD code FLUENT and its validation so that it can be used in performing the containment hydrogen distribution studies. In such studies, computational fluid dynamics simulations are necessary for obtaining accurate predictions. While steam condensation plays an important role, commercial CFD codes such as FLUENT do not have an in-built condensation model. Therefore, a condensation model was developed and implemented in the FLUENT code through user defined functions (UDFs) for the sink terms in the mass, momentum, energy and species balance equations together with associated turbulence quantities viz., kinetic energy and dissipation rate. The implemented model was validated against the ISP-47 test of TOSQAN facility using the standard wall functions and enhanced wall treatment approaches. The best suitable grid size and the turbulence model for the low density gas (He) distribution studies are brought out in this paper.

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1. Introduction

Large amounts of hydrogen could be generated and released into the containment during accident conditions in a typical nuclear power plant and its combustion may threaten the integrity of the containment. For the containment's integrity assessment, it is imperative that a detailed knowledge of the local distribution of hydrogen, steam and air inside the containment is necessary. Detailed description of flow patterns and gas distributions can be obtained through the CFD analysis. Further, these codes also allow users to integrate different models for simulating the basic phenomena. Steam condensation controls the steam presence in the containment in the medium and long term which affects the

mixing process and hence needs to be modeled. The commercial CFD codes do not have condensation models incorporated as a standard feature and this needs to be implemented before using it for hydrogen distribution analysis. The objective of this paper is to identify the best suited condensation model based on the available works and demonstrate that the chosen model is accurate and computationally efficient. In this direction, a best available condensation model was identified and implemented in the CFD code FLUENT. The condensation model implemented is based on Chilton–Bird formulations and is similar to the model presented by Arijit Ganguli et al. (2008) and Houkema et al. (2008). However, the validation details with regard to local behavior were not presented. This paper brings out the local behavior (temperature, velocities, species volume fractions, etc.) in addition to the global behavior. Houkema et al. (2008) used the diffusion coefficients which are determined for a constant temperature level and are kept constant during the calculation. The Fickian diffusion is valid when the mixture composition is not changing. Hence, the multi component diffusion treatment is used in this analysis. Malet et al. (2010) performed and compiled the

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Nomenclature

A, B, C	constants in Antoine equation
A_{wall}	wall surface area (m^2)
C_p	specific heat ($\text{J/kg}\cdot\text{K}$)
$C_{1\varepsilon}, C_{2\varepsilon}, C_{3\varepsilon}$	Constants
D	diffusion coefficient (m^2/s)
$\vec{F}$	force vector (N) or user defined sources
G_k	Generation of turbulence K.E. due to mean velocity gradients
G_b	Generation of turbulence K.E. due to buoyancy
G_ω	Generation of ω
$\vec{g}$	gravitational acceleration (m/s^2)
g_m	mass transfer coefficient ($\text{kg/m}^2\text{s}$)
h_i	species enthalpy (energy/mass)
$\vec{J}$	diffusion flux of species
k	kinetic energy per unit mass (J/kg)
k	turbulent kinetic energy (m^2/s^2)
k_{eff}	effective thermal conductivity (W/mK)
$\dot{m}$	mass flow rate (kg/s)
p	pressure (Pa)
q	heat flux (W/m^2)
R	net rate of production of species
S	user defined source
t	time (s)
T	temperature (K)
u, v	velocity (m/s)
$\vec{v}$	overall velocity vector (m/s)
w	mass fraction
x	steam mass fraction
Y	dissipation
Y_M	fluctuating dilatation in compressible turbulence to the overall dissipation rate
y	distance from the cell center to the wall (m)
y^+	dimensionless distance to the wall

Greek letters

ε	turbulence dissipation rate (m^2/s^3)
ν	kinematic viscosity (m^2/s)
ρ	density (kg/m^3)
$\bar{\tau}$	stress tensor (Pa)
σ	turbulent Prandtl numbers for k and ε
μ	dynamic viscosity (Pa-s)

Subscripts

cd	condensation
cell	in the center of the cell contiguous to the wall
cv	convection
f	condensate liquid film
i	interface
i, j	species
g	non-condensable gas
l	liquid phase
ref	reference
sat	saturated condition
w	wall
wall	at the wall
t	turbulence
h	heat
m	mass
k	turbulent kinetic energy
ε	turbulent dissipation
ω	specific dissipation rate

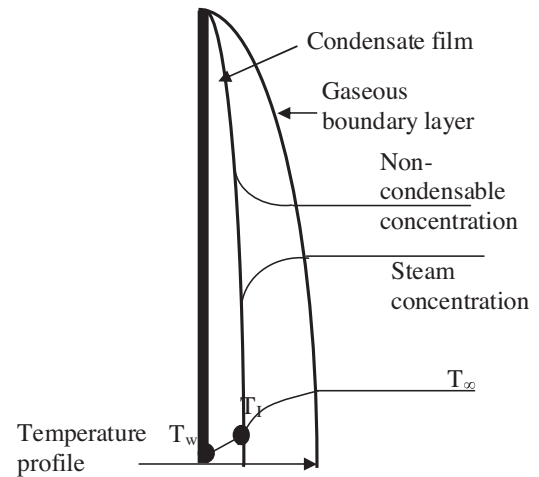


Fig. 1. Film condensation with non-condensables on a wall.

ISP-47 exercise on the validation of condensation models and recommended that the effect of mesh size (standard wall function and enhanced wall treatment) on the predictions should be studied for developing best practice guidelines. The present work deals with these two approaches and attempt to identify the best suited turbulence model and the grid for light gas distribution analysis. Such a model will be useful in formulating the best practice guidelines.

Many previous authors attempted to address the condensation in the presence of non-condensables. If one needs to model this process from first principles using mechanistic approach of heat and mass transfer, very fine computational grid is necessary near the condensation surface, which leads to long computational times for containment simulations. To reduce the computational time, [Klijanak et al. \(2006\)](#) have directly employed experimental correlations for condensation that have been obtained by Uchida. Other experimental correlations of Dehbi, Liu, etc. are also cited by [Rosa et al. \(2009\)](#). These correlations have been obtained to characterize the average condensation. The applicability of such correlations to predict the local behavior in containment is questionable. [Kudriakov et al. \(2008\)](#) have used Chilton–Colburn correlation based on heat and mass transfer analogy to characterize the local condensation. Gido-Koestel, Herranz, Pieterston, Kim and Corradini correlations based on heat and mass transfer analogy are also cited in the literature by [Arijit Ganguli et al. \(2008\)](#), [Houkema et al. \(2008\)](#) and [Malet et al. \(2010\)](#). The models that are based on heat and mass transfer correlations which were developed from integral experiments do not have a strong fundamental base as the bulk flow parameters appear in these correlations have been assumed to be the value in the wall adjacent node and hence depends on the computation grid used for a particular problem. The cells should be coarser for appropriate bulk flow parameters at the cost of the other important phenomena. The authors of these models also have pointed out this deficiency.

Film condensation process is shown schematically in [Fig. 1](#), where condensation takes place on the gas–liquid interface. Gradients of steam and non-condensables develop across the gaseous boundary layer ([Collier, 1972](#); [Incropera and DeWitt, 1996](#)). [Martin-Valdepenas et al. \(2005, 2007\)](#) developed a model in which liquid film resistance is considered. The liquid film heat transfer coefficient is obtained using Nusselt condensation model with correction factors for surface waviness ([Terasaka and Makita, 1997](#)). The heat flux due to condensation involves an empirical function obtained by fitting experimental data. The interface temperature is calculated iteratively. There are several effects that are not considered in the Nusselt liquid film theory which can affect the

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