NURETH14-406

VALIDATION OF THE CONDENSATION MODEL FOR CONTAINMENT THERMAL HYDRAULICS

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Abstract

The possibility of hydrogen combustion in reactor containments during accident conditions is one of the important safety issues. Experimental studies in the past have indicated that the steam condensation plays an important role in the hydrogen mixing and distribution in the containment. Computational Fluid Dynamics (CFD) simulations are necessary for accurate predictions. However commercial CFD codes do not have in-built condensation models. A condensation model has been developed and implemented in FLUENT computer code through user defined functions. The developed model has been benchmarked against a channel type geometry and ISP-47 test of TOSQAN test facility.

Introduction

Large amounts of hydrogen could be generated and released into containment during accident conditions in a typical nuclear power plant. The integrity of containment may be threatened by certain hydrogen combustion modes. The transport and distribution of hydrogen in the reactor containment in the presence of steam is one of the important safety issues. It is imperative that a detailed knowledge of containment thermal hydraulics is necessary to predict the local distribution of hydrogen, steam and air inside the containment. Internationally considerable efforts were undertaken to better understand the associated phenomena by conducting a large number of experiments. Nevertheless containment thermal hydraulics remains an open issue. To enable determination accurate hydrogen a multi-dimensional computational tool, such as Computational Fluid Dynamics (CFD) code, is necessary. However, the commercial CFD codes do not have condensation models incorporated as a standard feature.

A condensation model was implemented in the CFD code, FLUENT and benchmarked against predictions for the idealized version of the CONAN test facility. The paper also discusses the benchmarking of the numerical results with the experiments conducted in the TOSQAN facility, wherein helium distribution was measured in the presence of steam condensation.

1.0 Condensation model development

Film condensation with non-condensable gases can be represented by schematic as shown in Figure 1. Close to the wall is a layer of condensate film in which the temperature drops from that of the wall to the interface temperature. Following this condensate layer is the gaseous diffusion layer. Across the gaseous boundary layer, gradients of steam and non-condensable gases develop. In the present work the condensate layer is ignored, but the mass, energy and other associated turbulence parameters that goes into the film are accounted using sink terms.

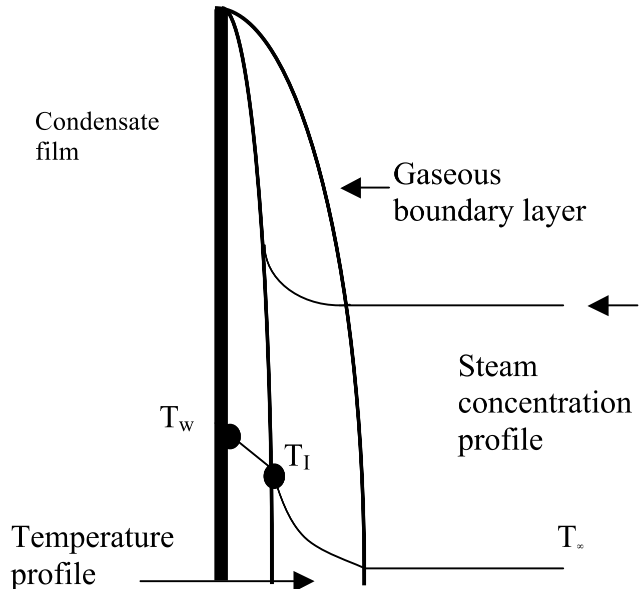

Figure 1 Film condensation with non-condensable gases on a wall

The condensation model incorporated in CFD code FLUENT through user defined functions (UDFs) is similar to NRG model [1]. The convective flow of gas occurs due to steam condensation at the wall. The mass balance of steam at the interface (subscript i) between gas and condensate film at the wall is:

Condensation flux = Steam transported through bulk motion + Diffusive transport

If the condensation flux at the wall is n_i, consequently, the bulk motion of the gas to the interface is equal to n_i as the film is impervious to non-condensable. In general, in a multi-component diffusion-convection the total flux consists of diffusion flux and convection flux. The diffusion flux near the wall can be represented through a mass transfer coefficient, g_m. The total flux of any species can then be represented by $x_i n_i + g_m (x - x_i)$, where x and x_i are the species mass fraction at the wall adjacent cell and at the wall respectively. The mass transfer co-efficient is a function of turbulence near the wall and is usually calculated by a CFD code internally. In the present case, as on the wall the total mass flux is the condensation flux, we can write:

$$n_i = x_i n_i + g_m (x - x_i) \tag{1}$$

The above equation can be reformatted as:

$$n_i = g_m \frac{x - x_i}{1 - x_i} \tag{2}$$

Numerically, this can be expressed as:

$$n_i = g_m \frac{x_{cell} - x_{wall}}{1 - x_{wall}} \tag{3}$$

Where, x = steam mass fraction
x_i = steam mass fraction at the interface

The mass fraction x_{wall} of steam at the surface of the condensate film at the wall is calculated from the vapour pressure at the surface. The Antoine equation is used to describe the vapour pressures as a function of the surface temperature:

$$\ln(p_{vap}) = A + \frac{B}{T + C} \tag{4}$$

The co-efficients A = 23.1512, B = -3788.02 K and C = -47.3018 K are fitted on data from steam tables. The mass of the steam that condenses has to be removed through a mass sink at the wall. The associated enthalpy sink is required to remove the enthalpy associated with the mass of steam condensed. It is assumed that the condensing wall immediately removes the condensation heat. The enthalpy sink Q for each cell is calculated by:

□=□□□□□□□□□□□□□□□□−□□□□ (5)

T_{ref} is the reference temperature (298.14 K) at which the enthalpy is zero. The turbulent quantities associated with this mass are also to be removed. The sinks of the turbulent quantities are calculated by:

Turbulent kinetic energy (k) sink is given by:

□□=□ □□□□□□□□□□□□ (6)

Turbulent energy dissipation rate (ε) sink is given by:

□□=□ □□□□□□□□□□□□ (7)

These mass, energy, turbulent quantities such as kinetic energy and energy dissipation rate and species sink (steam sink) are modeled using UDFs and implemented in the CFD code FLUENT.

2.0 Condensation on an isothermal plate

The benchmark exercise involves simulation of the condensation in a flow domain representing channel type geometry. The aim of this exercise was to compare with the correlation based on heat and mass transfer analogy for a classical problem of condensation on a flat plate.

$$Sh = 0.0296\, Re^{0.8} Sc^{0.33} \quad (8)$$

The University of Pisa proposed an initial step of the Benchmark (identified as the 0^{th} Step) aimed at comparing code responses among each other and with applicable correlations in the application to a classical problem of condensation on a flat plate. The reference geometrical and operating conditions for this step were selected as an idealization of the CONAN experimental facility operated at the University of Pisa [2].

2.1 Problem description

The geometrical configuration of the problem is shown in Figure 2. The left wall is maintained at a constant temperature (303.15 K) and the right wall is adiabatic wall where heat flux is zero. The fluid with a velocity of 3 m/s at a temperature of 363.15 K is assumed as an inlet condition.

The thermal conductivity and specific heat at constant pressure are assumed to be constant throughout the calculation. Density is computed from incompressible ideal gas law and viscosity is computed from the mixing law. For the present analysis, the Fickian diffusion approach is used. Diffusion coefficients used are obtained from the handbook of Vargaftik et al. (1975). The diffusion co-efficient of steam is obtained from air-steam system and a value of 0.3451 cm^2/s is used and kept constant throughout the calculation. The turbulence model k-ε is used. Near wall modelling is treated using enhanced wall treatment to resolve the viscous sub-layer.

2.2 Results and discussion

The grid sensitivity analysis was performed and it was found that the predictions are not sensitive for the grid size beyond 400x200. The wall y^+ values are in the range of 1 o 1.5. Ideally, the y^+ value should be around 1. However, up to a value of 5 can be used. Figure 3 shows the wall y^+ ($u^* y/\nu$) values obtained. The near wall mesh resolution is in the laminar sub-layer, for which the boundary layer can be resolved. Figure 4 shows the condensation mass flux along the wall. The mass flux varies from about 0.08 kg/m^2s to about 0.01 kg/m^2s along the height of the left wall.

Sherwood number is defined on the basis of computed condensation mass flux as

□ℎ□=□″□□□□□□□□□□−□□□□□

(9)

The local Reynolds number and Schmidt numbers are defined as [3]

□□□=□□ℎ□□□□□□ □ □□

(10)

□□=□□□□ (11)

Where □″ = mass transfer rate (kg/m^2s), ρ = density (kg/m^3), *D*= diffusion coefficient (m^2/s), ω = mass fraction of steam, ν = kinematic viscosity (m^2/s), □□ℎ□□□□□ = average channel velocity (m/s)

The analysis predictions using two definitions of sherwood number are compared with the correlation based on analogy between heat and mass transfer as shown in Figure 5. The predictions are in good agreement with the correlation. The legend 'predicted' indicates that the Sherwood number calcualted from the Eq. (10). The legend 'predicted – Eq.(13)' indicates that the Sherwood number is calcualted from the Eq. (12) as used by Ambrosini et al. is:

□ℎ□=□″□□□□□□ 1−□□□□□1−□□□□□

(12)

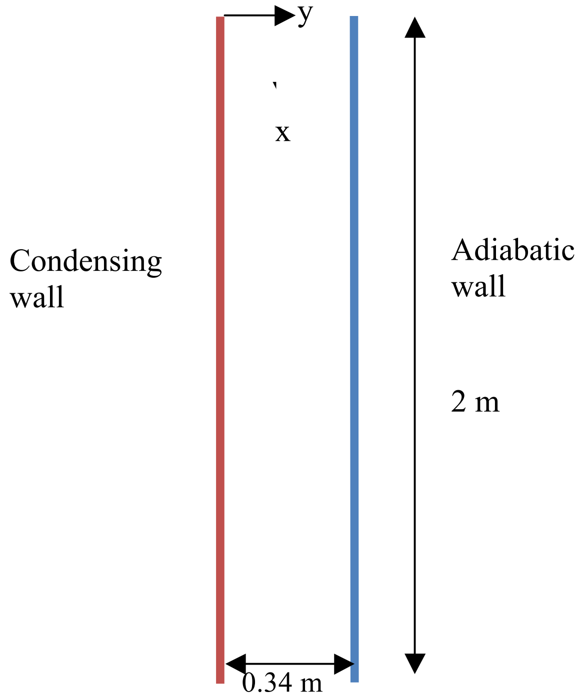

Figure 2 Geometrical configuration

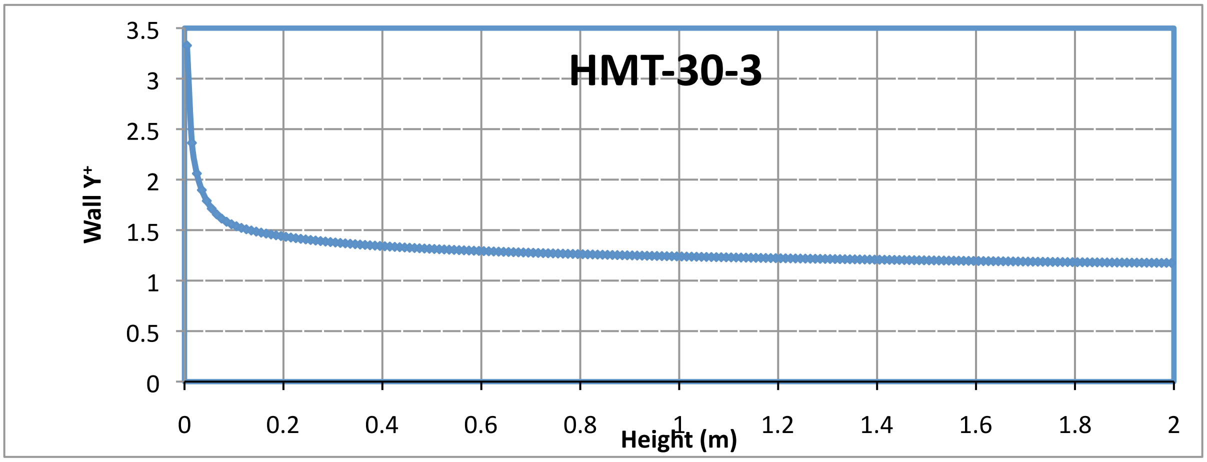

Figure 3 Wall y^+ (Left wall)

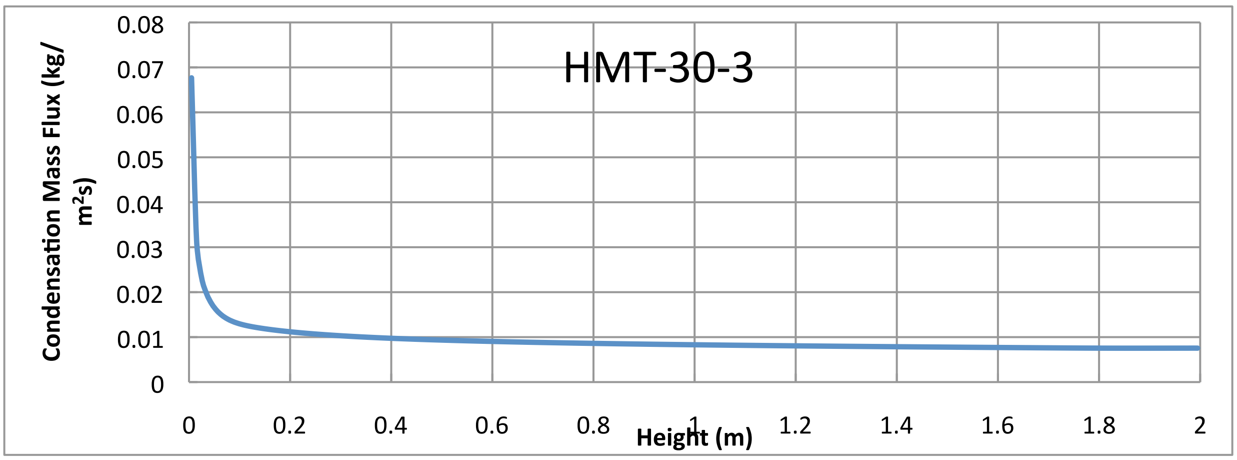

Figure 4 Condensation mass flux along the left wall

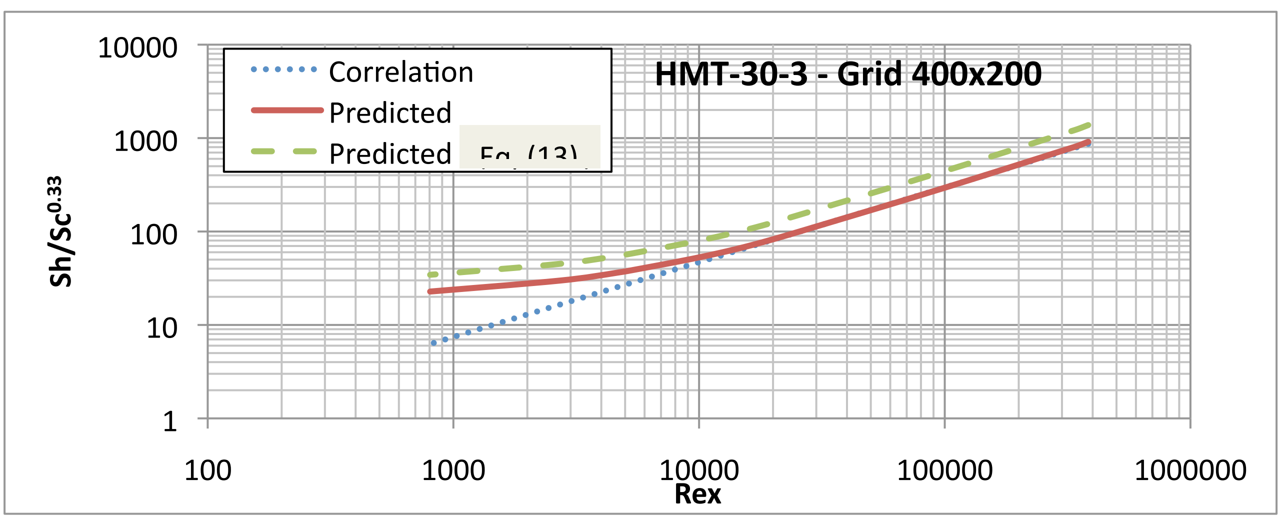

Figure 5 $Sh/Sc^{0.33}$ vs. local Reynolds number (HMT-30-3)

3.0 Simulation of TOSQAN facility

The experimental facilities such as TOSQAN (France), MISTRA (France), ThAi (Germany), multi-compartment experimental facility (South Korea) etc. have been used for the containment thermal hydraulic studies. Most of these experimental facilities are equipped with instrumentation for measurement of local temperature, species concentration and velocities. This enables a better understanding of mixing and stratification processes. Besides, local data may be used to assess the validity of simulations performed by CFD codes. [4].

The international standard problem exercise ISP-47 was launched to assess the capability of CFD and lumped parameter codes in the area of containment thermal hydraulics. The validation of TOSQAN test facility was a part of this ISP-47. Wall condensation and buoyancy are addressed under well-controlled initial conditions in a simple geometry in the TOSQAN test facility. The experimental data of TOSQAN test facility and its benchmarking results are presented by Malet et al., 2010 [5]. The TOSQAN facility was simulated using both the CFD codes [GOTHIC, TONUS, STAR-CD, CFX etc.] and lumped parameter codes [ASTEC, MELCOR, CONTAIN etc.] by numerous participants with different condensation models and turbulence models. The present study deals with the simulation and benchmarking of the TOSQAN experimental facility using the CFD code FLUENT to evaluate the condensation model and also to assess the behaviour of non-condensable gases.

3.1 TOSQAN

The TOSQAN facility is devoted to the study of different basic phenomena especially for the validation of field codes. The facility is a cylindrical vessel with an internal volume of 7.0 m^3 (Figure 6) [6]. The total height of the facility is 4.80 m, and the diameter of the main cylindrical part is 1.50 m. Steam and other gases are injected through a vertical tube of 41 mm inner diameter located at the vessel centre-line. The injection opening is located at the elevation 2.10 m with respect to the sump floor. The temperature of the vessel walls may be controlled so that the walls are divided into a “hot” zone and a “cold” zone. Steam may condense on walls located in the cold zone, where the controlled temperature is maintained at sufficiently low levels. Instrumentation was provided for measuring temperature and pressure, mass flow-rates, volume fractions etc.

Steam condensation occurred only on walls with lower temperature. The sump, where the liquid from the condensate film collected, was drained continuously. The test is composed of a succession of different steady states obtained by varying the injection conditions in the vessel as shown in Figure 7. Three steady states of air-steam mixture at two different pressure levels, and one steady state of air-steam-helium mixture were obtained. Each steady state is reached when condensation rate becomes equal to the steam injection flow rate. The objective of the two initial steady states is to produce two different kinds of flows by changing the injection mass flow rate. The objective of the third steady state is to test the influence of initial conditions in the numerical calculations. The objective of the fourth steady state is to test the numerical modeling with a non-condensable gas (helium) on the mixing, the mass distribution and the condensation [5].

3.2 Simulation

The simulation of the TOSQAN test facility is carried out by using CFD code FLUENT for the present study. Initial conditions before the steam injection, the injection flow rates of species viz. steam, air, helium and temperatures with time and the wall temperature characteristics for the condensing and non-condensing walls are obtained from the Malet et al., 2010.

User defined functions (UDFs) were developed for steam mass flow rate, air mean mass flow rate and helium mass flow rates as they are varying with the time. This was done by simulating the total mass flow rate of all species and mass fraction of individual species i.e., separate UDFs for mass flow rate and species. Similarly, the condensing wall temperature and injection mean temperature also varied with time during the experiment; hence separate UDFs were developed to simulate this.

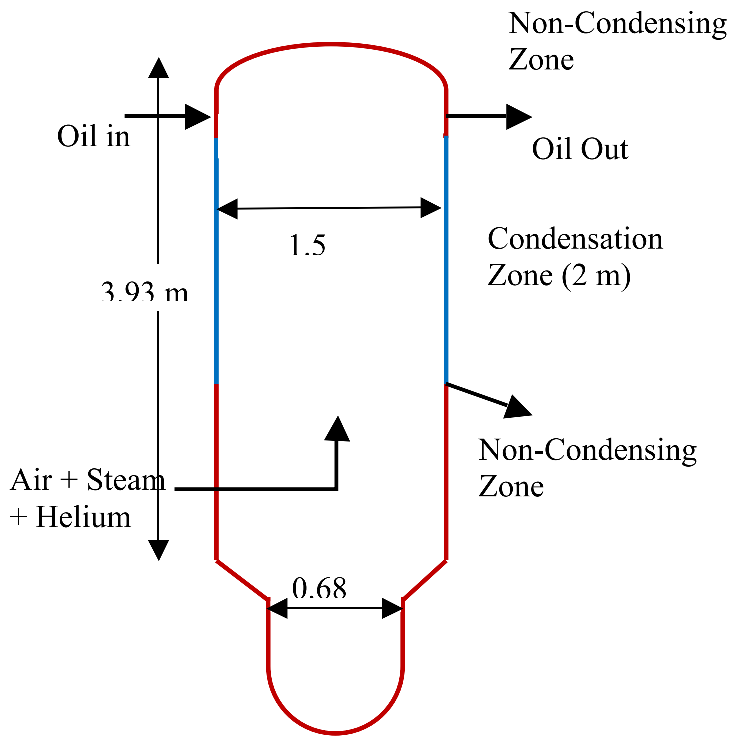

Figure 6 TOSQAN experimental facility [5]

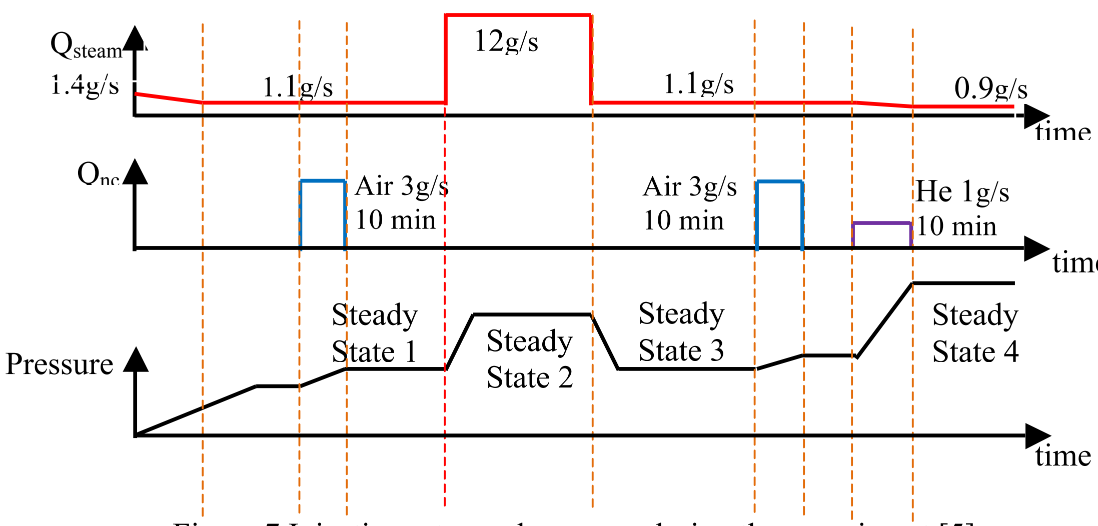

Figure 7 Injection rates and pressure during the experiment [5]

3.2.1 Geometric Model

The benchmarking of the TOSQAN test facility was carried out by about 10 participants as a part of the ISP-47 using CFD codes. A two-dimensional model was used by 8 participants and 2 participants used a three dimensional description of the experiment. A two dimensional axisymmetric model produced fairly good agreement with the experiment [1]. The experimental wall temperatures are regulated and central steam and helium injections take place, hence a 2-D axisymmetric model was applied for this study to reduce the computational time. The computational domain used for the present simulation is shown in Figure 8 and there are total of about 3586 cells considered in the flow domain. Twenty two nodes in the radial direction and 163 nodes in the axial direction are considered. The condensation zone from 2.391 m to 4.391 m includes 67 nodes in the axial direction.

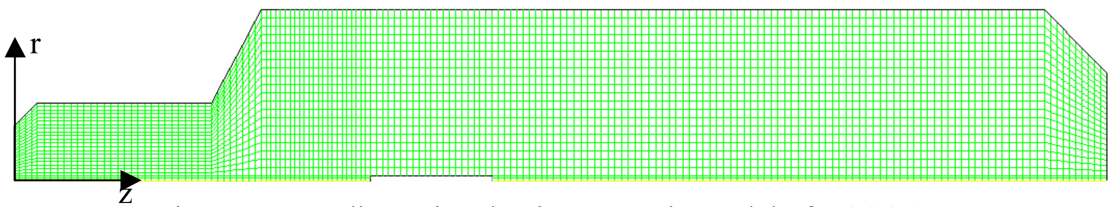

Figure 8 Two-dimensional axi-symmetric model of TOSQAN

3.2.2 Physical Model

The air-steam and air-steam-helium atmospheres are treated as single phase gaseous mixtures. The compressible flow model and k-ε turbulent models are used for the simulation. The k-ε turbulence model is used with standard wall functions. The floating operating pressure option is used in the simulation. This option handles time dependent compressible flows with an increase in the absolute pressure in the domain. The condensation model discussed in the previous section was incorporated in the FLUENT through user defined functions. Houkema et al., 2008 used the diffusion coefficients which are determined for a constant temperature level and are kept constant during the calculation. However, the multi component diffusion treatment is used in this analysis. Diffusion coefficients used are obtained from the handbook of Vargaftik et al. (1975)[7]. The mixture diffusion co-efficients are calculated from the user supplied binary diffusion coefficients. A constant value of diffusion co-efficient for the steam in air-steam binary mixture is used. Similarly, a constant value of diffusion co-efficient for the steam in steam-helium binary mixture is used. Diffusion-coefficient of air obtained from air-helium binary system is used.

3.3 Results and discussion

The simulation is continued as per the simulation timings specified by the Malet et al., 2010.

3.3.1 Global Behaviour

Figure 9 shows the time-history of predicted and experimental (TOSQAN) values of pressure evolution during the test. The trends are in good agreement with the experimental values. However, there are slight differences in steady state magnitudes.

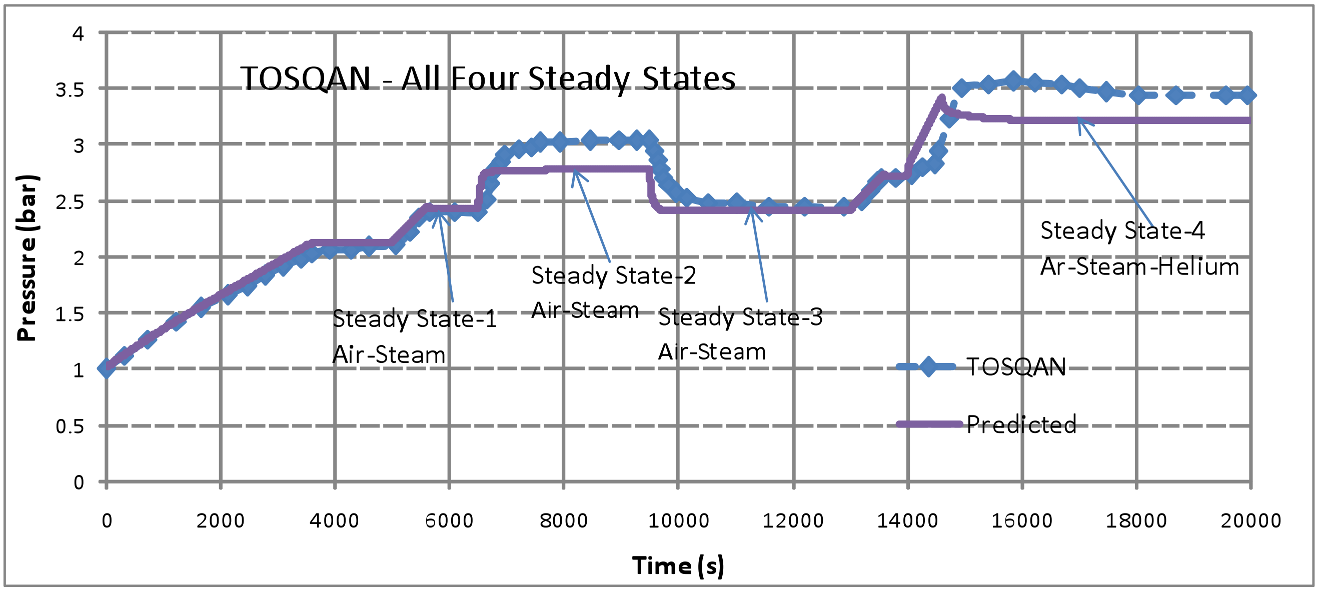

Figure 9 Pressure evolution during the test

3.3.2 Local behaviour

Parameters such as vertical and radial components of gas velocities, temperatures, mole/volume fractions of steam/helium for steady states 1, 2 and 4 are compared with the experimental data. Since axisymmetric model is used, the predictions of radial profiles for various parameters are available and plotted only from 0.0 to 0.75 m against the experimental data of -0.75 m to 0.75 m.

Steady State 1: The vertical component of gas velocity (Figure 10) is in agreement with the measured data. The vertical profile of the gas temperature is also in good agreement with the measured value as shown in the Figure 11. However, there are slight differences in trends and magnitudes as shown.

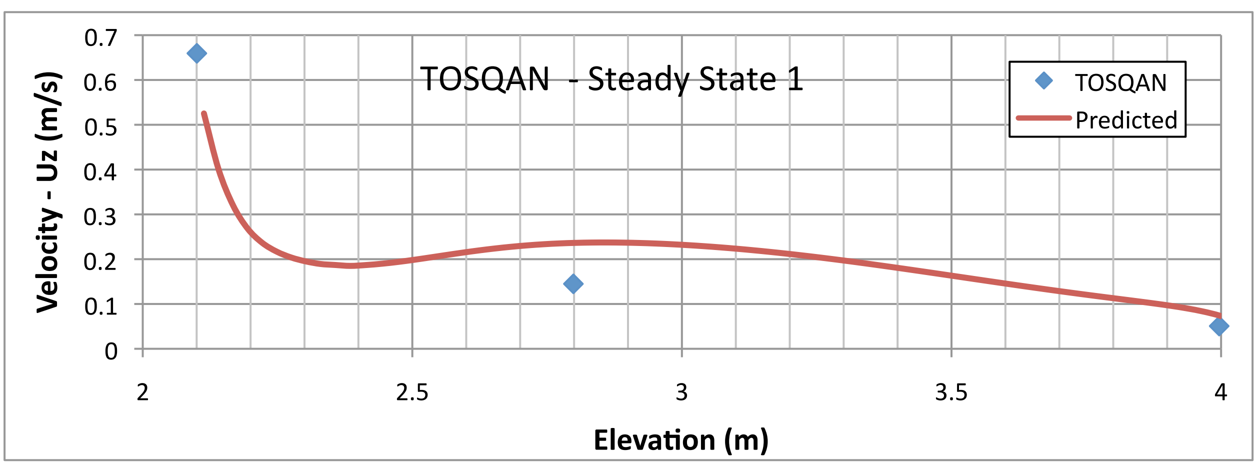

Figure 10 Vertical component of gas velocity during steady state 1

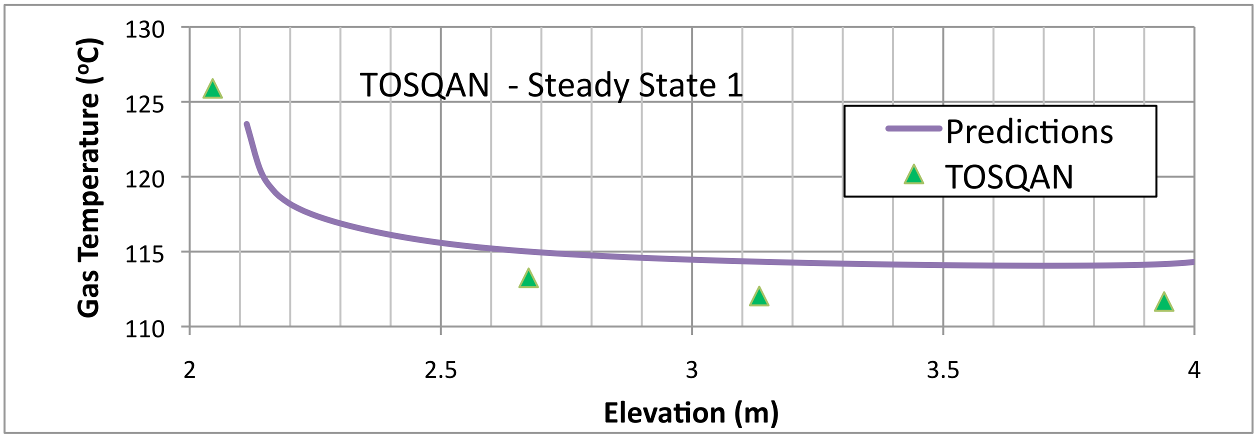

Figure 11 Gas temperature during steady state 1

Steady State 2: The vertical and radial components of gas velocity are in good agreement with the measured data as shown in Figures 12 and 13 respectively. The negative values of velocity could not be predicted at this location. Figure 14 shows the radial profile of the steam volume fraction. The trends of the predictions for the radial profile of the steam volume fraction are in good agreement; however, the magnitudes are having slight differences.

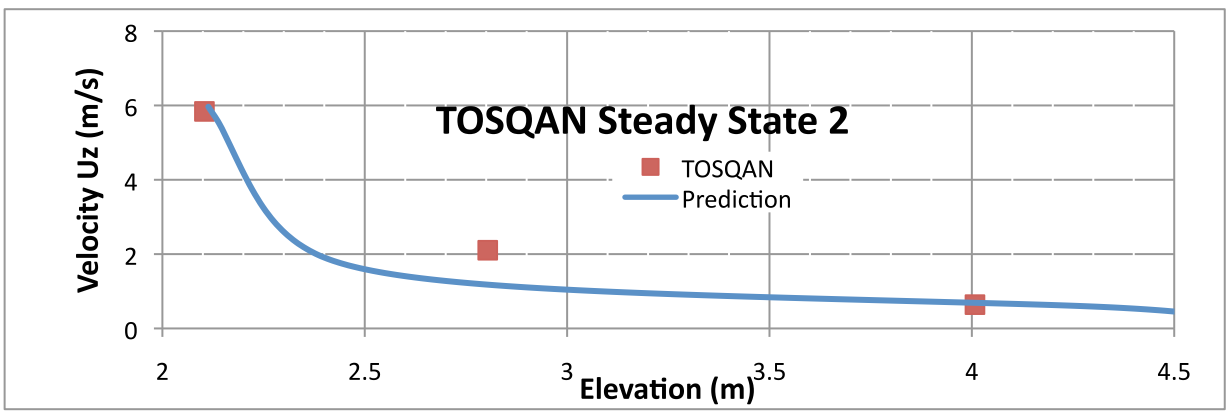

Figure 12 Vertical component of gas velocity during steady state 2

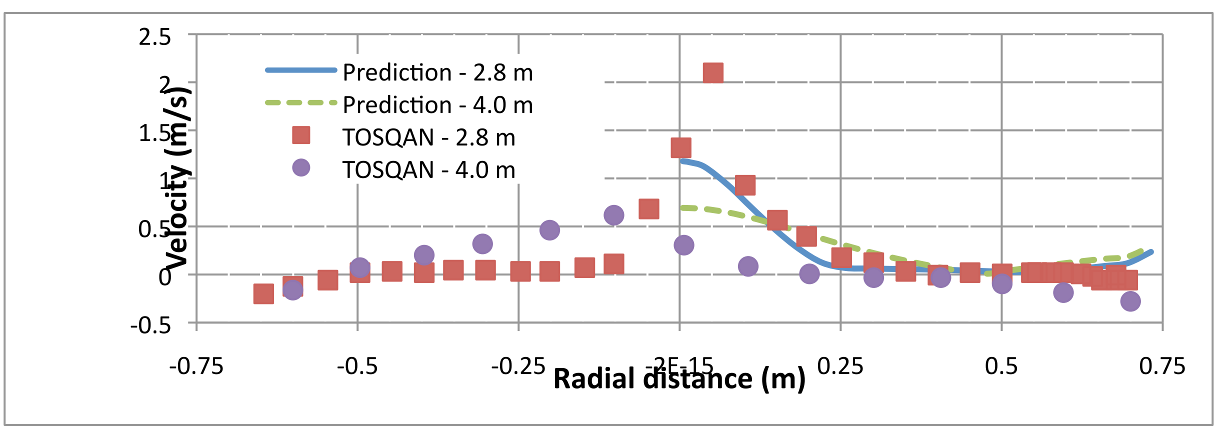

Figure 13 Radial profile of gas velocity during steady state 2

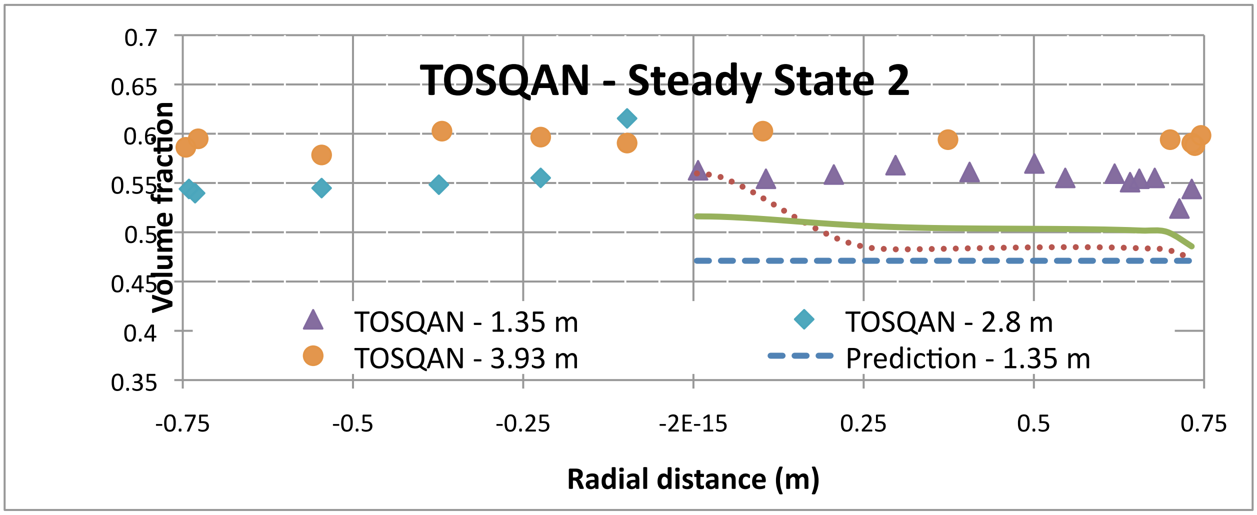

Figure 14 Radial profile of steam volume fraction during steady state 2

Steady State 4: The trends and magnitudes of the vertical and radial profiles of gas temperature distributions are in good agreement with the experimental data as shown in Figures 15 and Figure 16 respectively. The radial profiles of steam and helium volume fractions at three different locations are shown in Figures 16 and 17 respectively. The steam fraction is slightly under-predicted, whereas the helium fraction is slightly over-predicted.

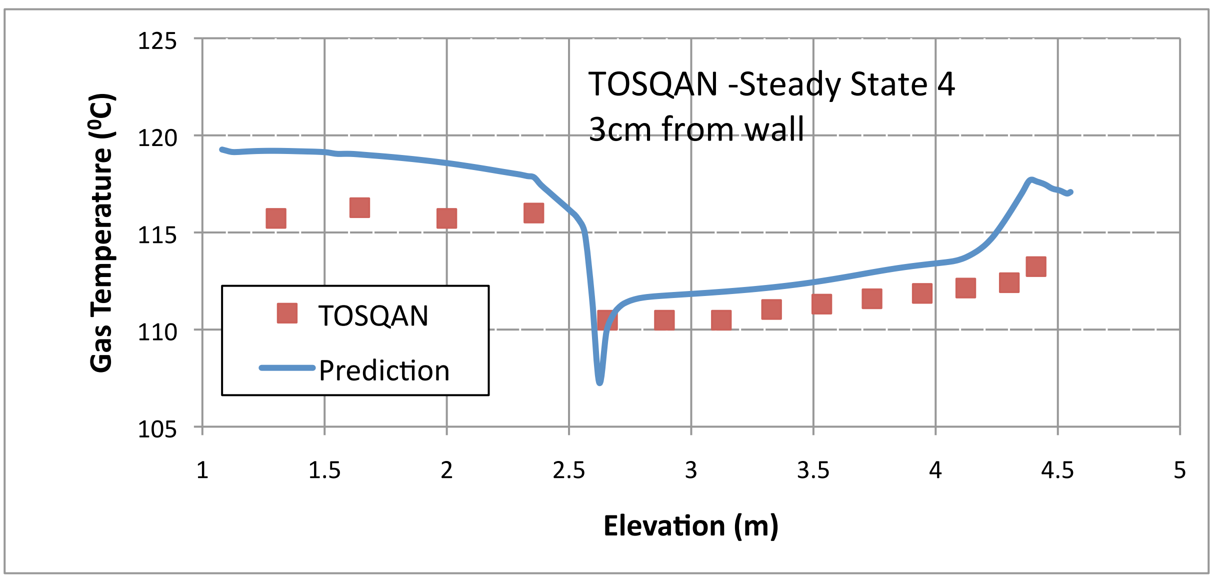

Figure 15: Gas temperature from 3 cm from the wall during the steady state 4

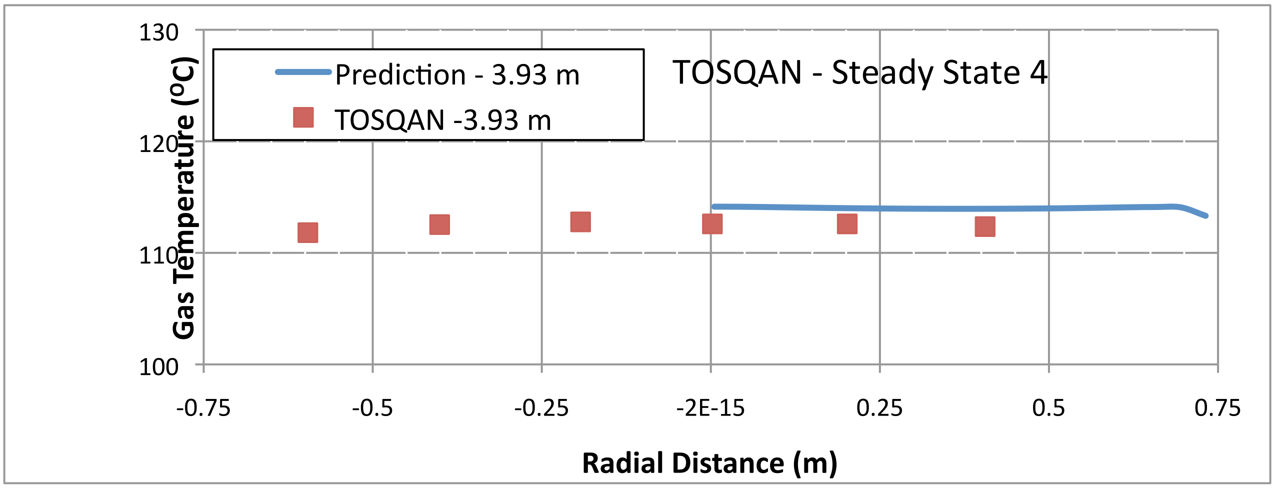

Figure 16 Gas temperature radial profile during the steady state 4

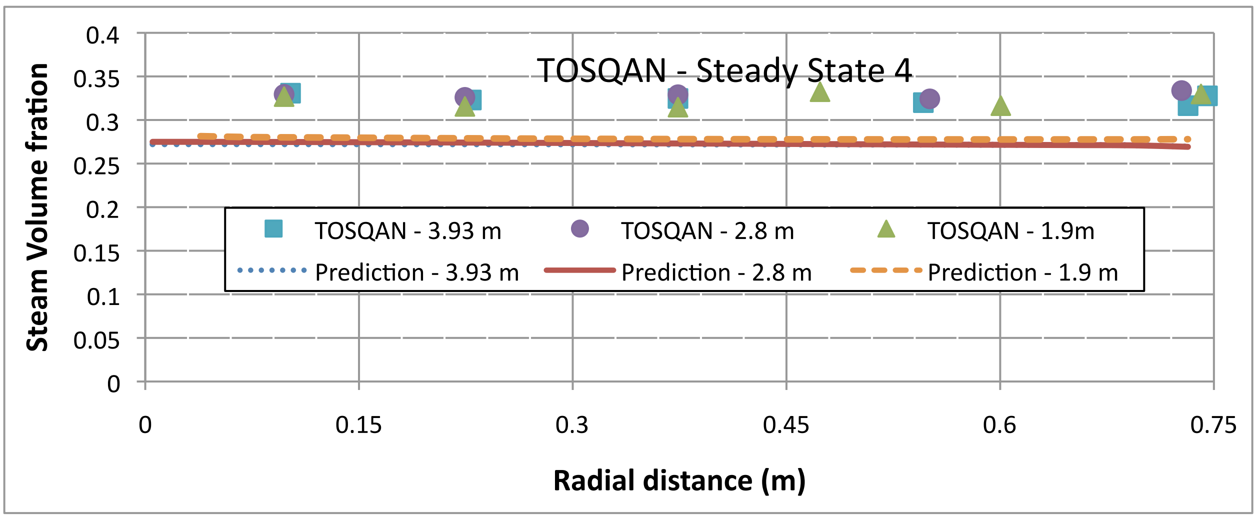

Figure 17 Radial profile of steam volume fraction during the steady state 4

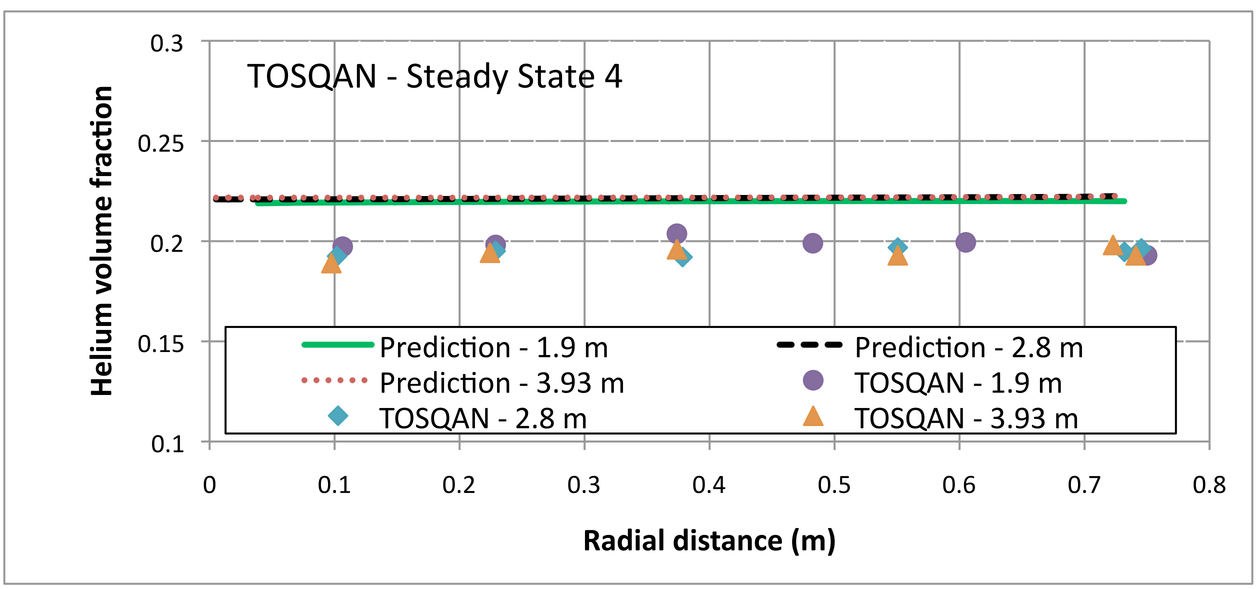

Figure 18 Radial profile of helium volume fraction during the steady state 4

4 Conclusion

A condensation model was developed and incorporated in the FLUENT CFD code through user defined functions. The model was benchmarked against the idealized version of the CONAN test facility. The predictions were compared with the correlation based on heat and mass transfer analogy. The predictions are found to be in good agreement. The ISP-47 test of TOSQAN test facility was simulated using the CFD code. The local and global behaviour is in good agreement with the measured parameters except for few minor variations in the magnitudes. However, local behaviour for some parameters is not in good agreement with the data. This is currently being looked into.

5 References

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