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THE APPLICATION OF CFD TO VENTILATION CALCULATIONS AT YUCCA MOUNTAIN

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ABSTRACT

This paper presents the results of the application of CFD to ventilation calculations at Yucca Mountain using MULTIFLUX. Seven cases were selected to study the effect of the heat transport coefficient on the drift wall temperature distribution. It was concluded that variable heat transport coefficients such as those given by the differential–parameter CFD used in MULTIFLUX are considered the most appropriate approach of all cases presented. This CFD model agrees well with FLUENT results and produces the lowest temperature results, which is favorable to ventilation performance.

INTRODUCTION

Hydrothermal-ventilation analyses are being conducted using MULTIFLUX 1.1 with embedded NUFT Version 3.0s [1] to predict temperature and relative humidity variations for three hundred years along the length of a selected drift at the center of the conceptual repository at Yucca Mountain (YM).

The heat and water movements caused by ventilation affect the YM barriers and are inputs to the Engineered Barrier System (EBS) Process Model.

MULTIFLUX is a coupled hydrothermal - ventilation numerical simulation software package designed to calculate time-dependent heat, moisture, and ventilation air fluxes in and/or around a subsurface opening. The drift (or airway) model-element includes the heat and mass transport between the nuclear waste packages, ventilating air, and the drift wall, using Computational Fluid Dynamics (CFD) heat and mass transport solvers. MULTIFLUX includes two CFD components, one for heat and one for moisture transport calculation. Significant sensitivity of the drift wall and waste package surface temperatures to the heat transport coefficients was found in a previous paper [2]. The aim of this paper is to study the relationship between the heat transport coefficient distribution on the emplacement drift and waste packages surfaces, and the temperature variations along the surfaces in the airflow direction.

THE MULTIFLUX VENTILATION MODEL

The method of the present analysis is to conduct ventilation calculations with a differential parameter (eddy diffusivity) CFD model in MULTIFLUX to simulate computational heat transport coefficient distribution on the waste package and wall surfaces. In addition, FLUENT [3] is used for comparison. Four computational cases (Cases I-IV) are selected to compare heat transport coefficient distributions for ventilation calculations. The coefficients are dependent on the temperature variation of the surfaces in the thermally developing turbulent flow. For the comparison three additional cases (cases V through VII) are used with simplified heat transport models. The summary of the basic input parameters used in the study is as follows:

Rock input data:	NUFT Version 3.0 input deck specified in the Multiscale Thermohydrologic Model [4] (MSTHM).
Drift dimensions:	600 m long, 5.5 m in diameter, according to MSTHM.
Ventilating air:	10 m^3/s at 25°C intake temperature with 30% relative humidity.
Waste packages:	Eight WPs in a repeating drift segment of 35.5 m according to MSTHM; 17 sections.
Areal mass load:	56 MTU/acre.

Computational Heat Transport Model Comparison

The input parameters result in turbulent flow in the drift with Re = 112,940. Other relevant input properties are as follows:

Specific heat of fluid at constant pressure	$c_p = 1006.44$	(J/kg·K)
Prandtl Number	Pr = 0.71	
Density	$\rho = 1.1665$	(kg/m^3)
Thermal Conductivity	$k = 0.026487$	(W/m·K)
Kinematic Viscosity	$\nu = 1.87\times10^{-5}$	(kg/m·s)
Pressure	$p = 88720$	(Pa)
Fluid Mean Axial Velocity	$u_m = 0.463652$	(m/s)
Physical Parameters:		
Inner Radius	$r_i = 0.835$	(m)
Outer Radius	$r_o = 2.75$	(m)
Number of radial divisions between the WP & DW	60, non-equally spaced	
Length of a drift section:		
Case I and II	150	(m)
Case III	35.5	(m)
Case IV	17×35.5= 603.5	(m)
Number of Sections:		
Case I, II, III	1	
Case IV-VII	17 (603.5 m total length)	

Method and Domain for Case I and Case II:

These two cases are used to compare results from (i) MULTIFLUX differential CFD, (ii) FLUENT, and (iii) experiments. The boundary conditions for these cases are (i) inside wall is kept at constant temperature, outside wall is unheated, and (ii) outside wall is kept at constant temperature, inside wall is unheated.

a) MULTIFLUX calculations

Fig. 1 shows a drift section for the MULTIFLUX Differential Parameter CFD calculations. The drift section is 150m long and has 50 segments of 3m each. There are 60 unequally spaced segments along the radius. The flow is assumed to be fully developed hydraulically when entering the drift section. The eddy diffusivity and the velocity profiles are given in the dimensionless equations by Kays and Leung [5]. These eddy diffusivity and velocity profiles are input parameters in the energy equation for heat transport calculation in turbulent flow. The energy equation, a second-order partial differential equation, is solved by MULTIFLUX to calculate the heat transport coefficient (h) for constant wall-temperature boundary condition.

b) FLUENT calculations

The goal of the FLUENT calculation is to provide values for comparisons in studying convective heat transfer characteristics in turbulent flow in a concentric annular drift. FLUENT 5.5 was used in the study. The computational domain for FLUENT is shown in Fig.1.b

Temperature and heat flow distributions were calculated in a drift with a length of 300 meters of which an unheated leading section of 150 meters was used to allow velocity profile development under isothermal condition. A step change in temperature was applied over the heated section. A mesh grid was defined with 0.5 meter axial and 0.095 meter radial sizes.

Case III: A Comparison Case

This case is used to compare MULTIFLUX with FLUENT when both walls are heated using variable temperatures over the surfaces in the flow direction.

a) MULTIFLUX calculations

There is only one drift section included in this case, shown in Fig. 1.c. The length of the section is 35.545m. There are 21 segments along the axis that are variable in length, corresponding to half WP lengths and to the small gaps between the WPs. There are 60 segments of variable length along the radius. The discretization of the length along the axial direction and the radial direction is shown in Tables I and II, respectively.

b) FLUENT calculations

The total length used was 185.5m, shown in Fig. 1.d. The first 150 meters were used as developing region for the air flow. The next 35.5m section was divided in 21 axial segments identical to those used in MULTIFLUX.

Table I. Discretization of the Length along the Axial Direction

Division	Length	Division	Length
1	1.865	11	0.1
2	0.1	12	2.6525
3	2.6375	13	2.6525
4	2.6375	14	0.1
5	0.1	15	2.6375
6	2.6525	16	2.6375
7	2.6525	17	0.1
8	0.1	18	2.6525
9	1.865	19	2.6525
10	1.865	20	0.1
		21	2.785

CALCULATION RESULTS

Case I, Verification

This case had two conditions:

a. Inside wall is kept at 50°C, outside wall unheated.
b. Outside wall is kept at 50°C, inside wall unheated.

Three different heat transport models were used under these conditions:

– Experimental heat transport coefficient correlations for circular annulus
– MULTIFLUX Differential Parameter CFD sub-model
– FLUENT

The results are shown in Fig. 2 a and b.

Case II, Comparison, Constant Temperature

In this case both the inner and the outer walls were kept at a constant temperature of 50°C. There are no experimental data available for this case. The computational results are shown in Fig. 2 c.

Case III, Comparison, Varying Temperature

In this case, both walls are heated and maintained at axially-varying temperatures which were determined from a preliminary MULTIFLUX calculation assuming an axially constant value of heat transport coefficient of 1.37 W/(m²K) for the inner and outer walls. The result of heat flux density values compares well with the FLUENT results. The results, however, are not shown here for the sake of brevity.

The run time for variable temperature for first section at the fifth time period using the MULTIFLUX Differential Parameter CFD was 14 seconds, with a 1.7 GHz Pentium IV processor. FLUENT was run on a SGI workstation and took about 2 minutes to complete the calculation.

Table II. Discretization of the Distance along the Radial Direction

Division	Length	Division	Length
1	0.835	31	0.149293
2	5.03×10^{-07}	32	0.167838
3	3.81×10^{-06}	33	0.145884
4	1.56×10^{-05}	34	0.126157
5	4.53×10^{-05}	35	0.108504
6	0.000106	36	0.092772
7	0.000215	37	0.078817
8	0.000393	38	0.066499
9	0.000664	39	0.055686
10	0.001058	40	0.04625
11	0.001604	41	0.038067
12	0.002341	42	0.031023
13	0.003307	43	0.025005
14	0.004546	44	0.019909
15	0.006104	45	0.015636
16	0.008034	46	0.012091
17	0.010389	47	0.009187
18	0.013228	48	0.006842
19	0.016614	49	0.004977
20	0.020612	50	0.003523
21	0.025293	51	0.002415
22	0.03073	52	0.001592
23	0.037	53	0.001
24	0.044184	54	0.000592
25	0.052368	55	0.000324
26	0.06164	56	0.00016
27	0.072093	57	6.82×10^{-05}
28	0.083822	58	2.35×10^{-05}
29	0.096929	59	5.73×10^{-06}
30	0.111516	60	7.58×10^{-07}

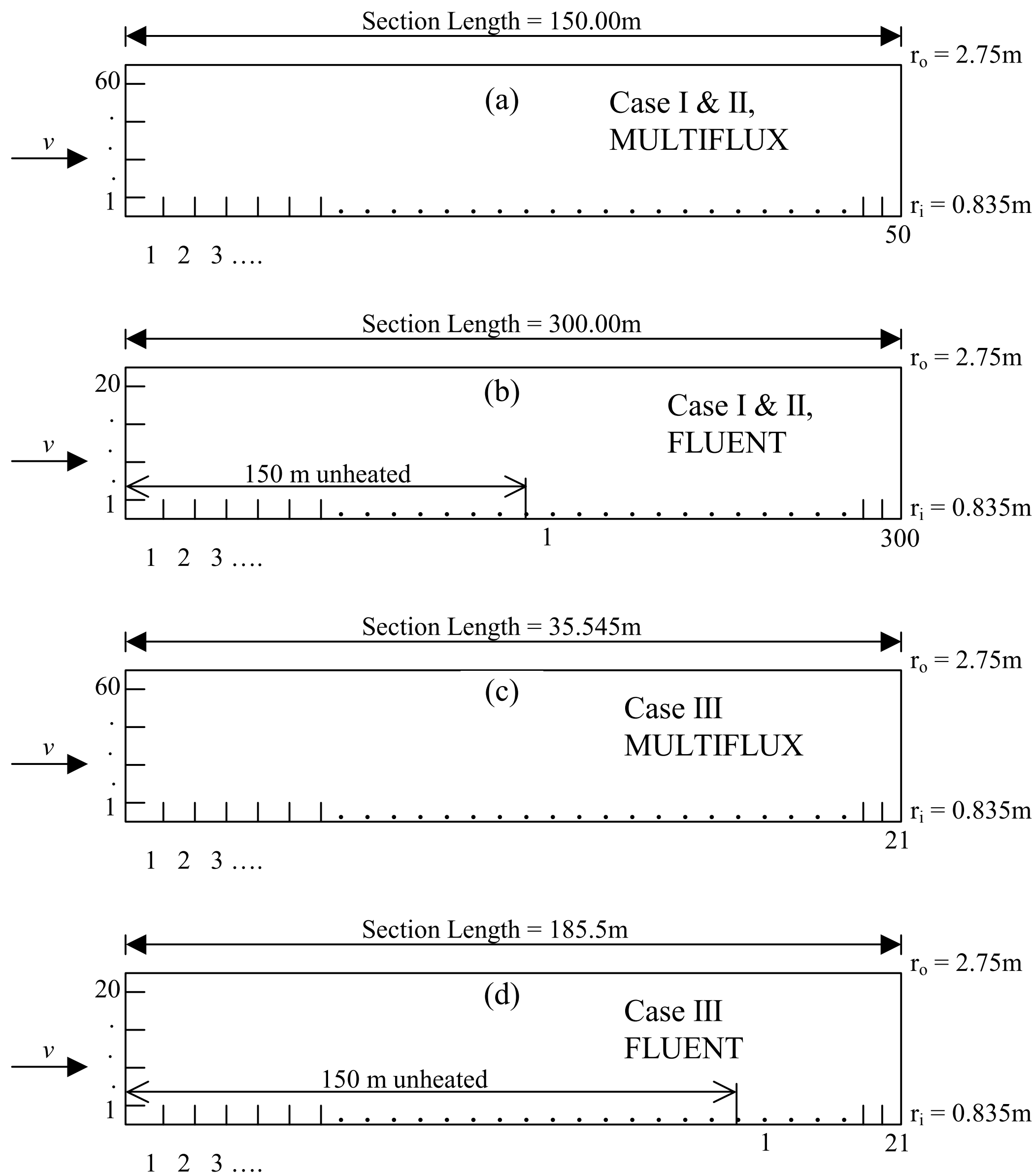


Fig. 1. Drift Sections used in cases I-III in MULTIFLUX

Application of MULTIFLUX V1.0 differential parameter CFD to ventilation calculation

Four additional cases were prepared to study the effect of the variable heat transfer coefficient on the drift wall temperature. The calculation domain includes a full drift length of 603.5 m. Results are presented as a function of both time and position for cases IV-VII. A non-uniform waste package heat load was used in the MULTIFLUX calculations.

Case IV: In this case, variable heat transfer coefficients, calculated by the differential parameter CFD are used. The heat transport coefficient variations are iteratively calculated, over time and space for a full drift as a function of inner and outer wall temperatures. The corresponding temperature distributions and heat transport coefficients of time and position are given in Fig. 3.

Case V: In this case, constant heat transfer coefficients (inner wall hi=1.84, outer wall ho=1.33), obtained from averaging the variable coefficients of Case IV, are applied to ventilation calculation.

Case VI: In this case empirical constant heat transfer coefficients (inner wall hi=1.59, outer wall ho=1.15) are used in the ventilation calculation. These coefficients are obtained from an empirical heat transfer model specifically developed for turbulent flow in a circular annulus with walls kept at a constant temperature, according to Kays and Leung [5].

Case VII: In this case, an AMR- equivalent heat transfer coefficient of Dittus and Boetler [6] of 1.37, based on airflow in equivalent circular duct, is applied to ventilation calculation.

Figure 4 shows the graphical presentation of the results for the 1st and 17th sections for the fifth time interval by comparing cases IV through VII.

CONCLUSIONS

Four models are compared to study the effect of heat transport coefficient variability on the drift wall temperature distribution. Case VI may be considered as a reference model since it is experimental-empirical and specifically obtained for a circular annulus. This model gives the highest temperatures for the duct wall. However, the correlation conditions (i.e., the assumption of thermally developed flow with constant wall temperatures) are not applied in these cases.

Case VII uses the Dittus-Boelter experimental-empirical model, and it results in similar temperatures to those of Case VI. However, the correlation conditions are violated not only by the variable-temperature boundary but also by the geometry which is not a simple circular duct but an annulus.

Case IV uses the MULTIFLUX differential parameter CFD results, based on an experimental-empirical eddy-diffusivity model specifically determined for circular annular duct flow. The CFD model agrees with experimental results published for heat transfer in annular duct flow (Case I). Therefore, variable heat transport coefficients such as those of Case IV are considered the most appropriate approach of all cases presented. This CFD model produces the lowest temperature results, which is favorable to ventilation performance.

Case V is closer to Case IV than the other cases. It is based on using the average of the Case IV variable heat transport coefficients, rather than constant values obtained by other means. However, the difference between the variable coefficient and constant coefficient results is still significant. This observation quantifies the value of using variable, instead of averaged, heat transport coefficients in ventilation calculations.

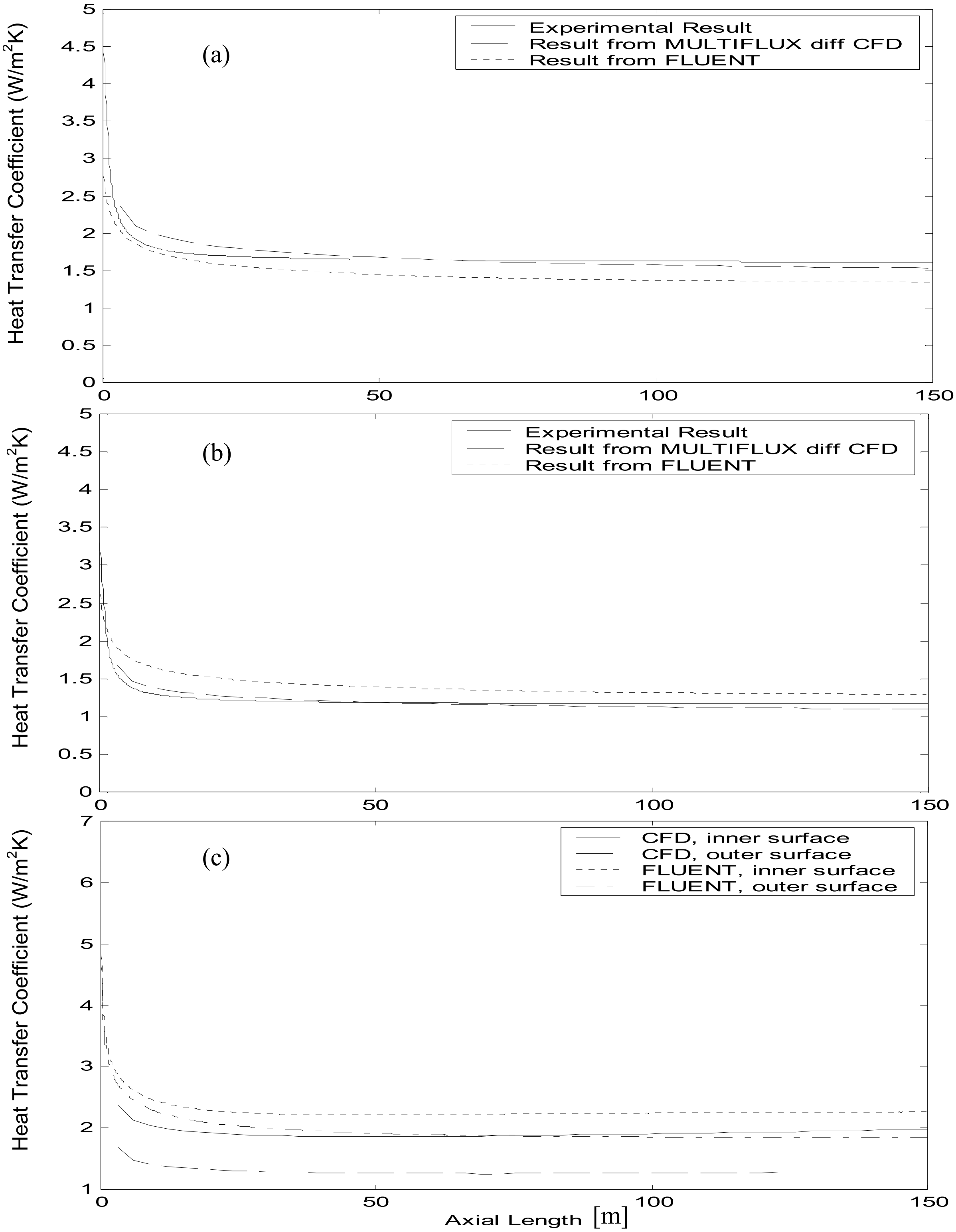


Fig. 2. Comparison of Heat Transport Coefficient variations (a) Heated inner surface and unheated outer wall (b) Unheated inner surface and heated outer wall (c) Heated inner and outer wall

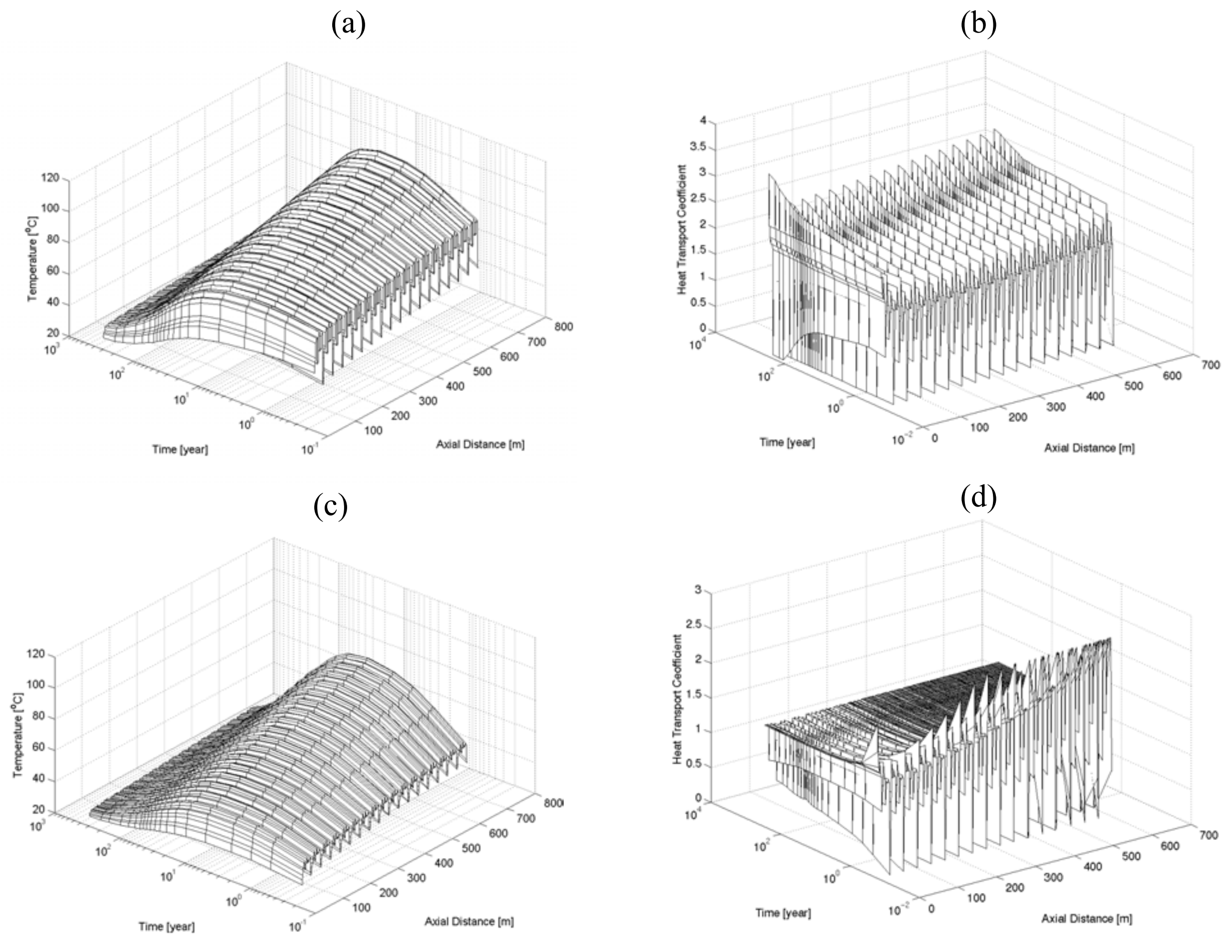
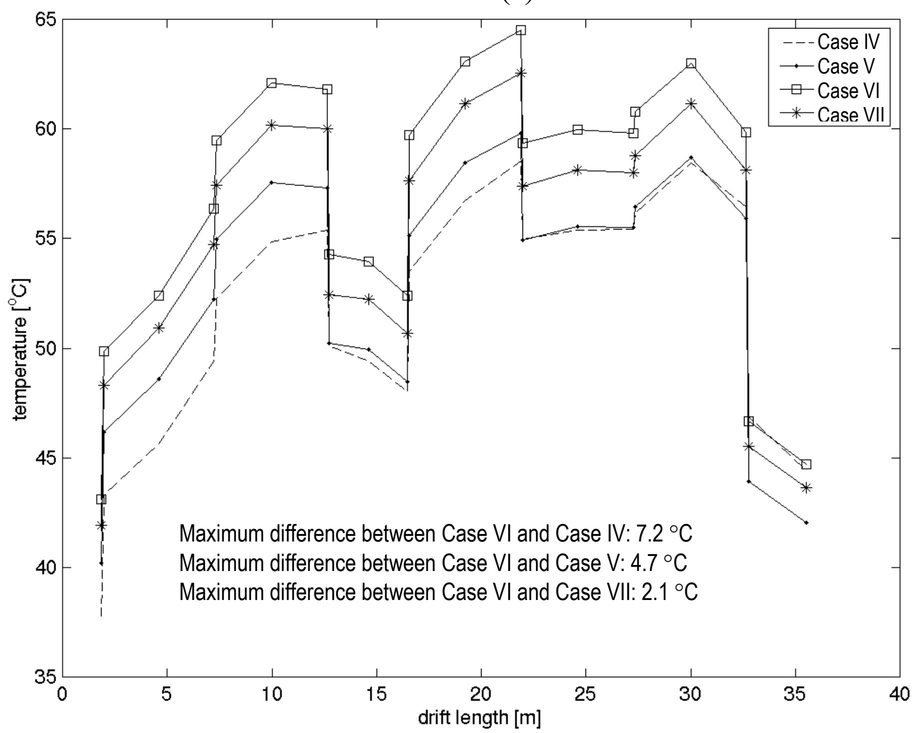


Fig. 3. Corresponding temperature and heat transport coefficient distributions, (a) temperature distribution at the inner wall, (b) , heat transport coefficient on the inner wall, (c) temperature distribution at the outer wall and (d) heat transport coefficient on the outer wall.

(a)



(b)

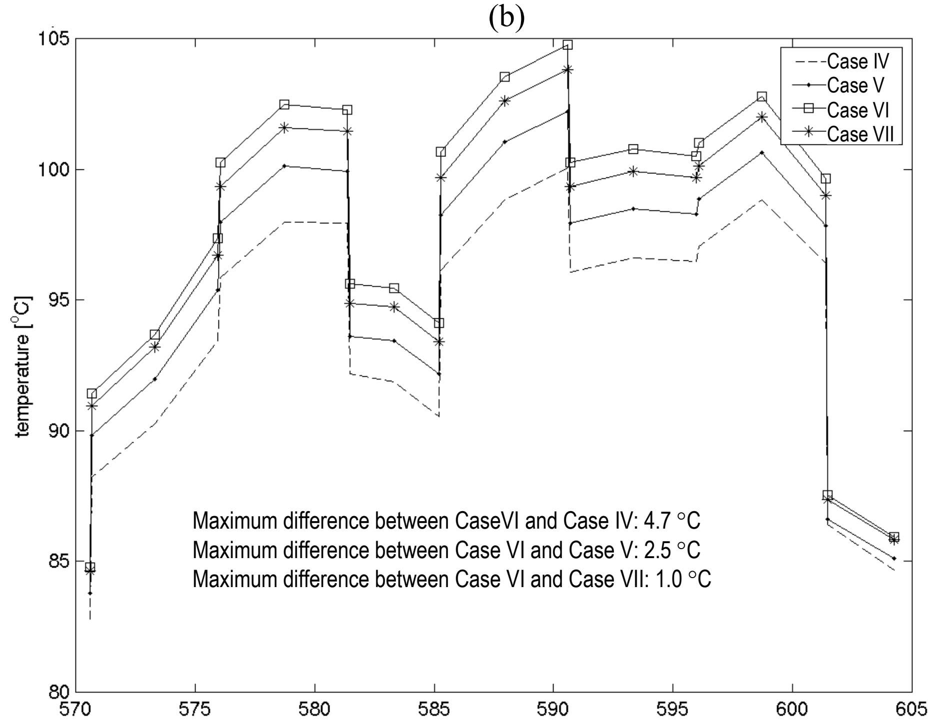


Fig. 4. Comparison between the cases IV- VII: (a), first drift section; (b), 17th drift section

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