

Fiscal Year-End Report

Radiation Characterization Procedure and Thermo-mechanical Design of High Temperature Compact Heat Exchanger for Combined Power Generation Cycle

Submitted by

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Abstract

This report presents the end of fiscal year documentation of the assigned tasks by the Zero-Emission Technology Group, CANMET Energy Technology Centre-Ottawa. The tasks entailed the preliminary review of both the radiative heat transfer characteristics from a combustion chamber and the procedure towards the design of compact heat exchanger. The challenges encountered due to lack/provision of basic design tool for numerical modeling procedure necessitated the evaluation of Energhx Consulting's flow-solver. The integration of this solver with the development framework of graphic user-interface and visualization, towards developing a customized Window-based Application for each of these tasks, were discussed.

The procedure adopted towards developing the software application can be used as design methodology for the assigned task and other future numerical modeling tasks within the group. This involves the use of flow-solvers, known as PlainFlow[®], for possible incorporation into the software development package. Also, this report includes the presentation of a brief literature reviews for both the radiative characteristic and compact heat exchanger modeling. While the detail about former is limited to the review outlined in chapters 1 & 2 (since the task was discontinued after three months into the review and set-up procedure), the report contains the detail implementation procedure of the latter task.

Preliminary results of developing entropy boundary layer and flow characterization results will be discussed. Also, recommendation for future work with or without the use of the flow-solvers from Energhx Consulting will be presented.

1. INTRODUCTION

Rising demands for increase in the generation of clean energy from power plants have enabled growing interest in the development of innovative heat recovery systems and combined cycles. Existing power generation schemes that have been considered for large-scale capture of CO₂ include oxygen combustion and flue gas approaches, which actually involve the treatment of the resulting flue gas from the combustor for separation. These flue gases carry high quality of heat energy which can be recovered before the separation procedure. Therefore, there is an opportunity to develop and integrate new power cycles, which may offer higher efficiencies to the existing combustion cycle. The background of two major tasks towards solving the challenges of developing an efficient integrated power cycle is presented in this chapter.

1.1 Background

The design of thermofluid systems, upon which all energy systems involved in combined power generation cycle are based, depend on the modeling of the transport of constituent mass and heat quantities within the system. The complexities of these models will depend on the nature of constituency flows, the boundary and the operating conditions. While adequately set-up experimental techniques represent consistent modeling tool, by producing more reliable physical data; these techniques can be prohibitively expensive and time consuming. Since the advent of computers, numerical modeling of complex problems provides an alternative effective tool for product development. Consequently, the design cycle approach involves the use of experimentally validated numerical model for the development of all energy system components.

The physics of all heat and mass transfer problems are constituted by the Navier-Stokes equations, comprising the understanding of the conservation of mass, the conservation of momentum, and the conservation of various energies or conversion of energies within the energy system under consideration. Consequently, both the modeling of the radiative heat transfer characteristics and the thermo-mechanical design of compact heat exchanger are dependent on stable and accurate flow-solvers (a numerical module that solves the discretized governing equations of mass and heat). Popular flow-solver algorithms include the Finite Element Method (FEM) and the Finite Volume Method (FVM), in addition to Finite Difference Method (FDM). Most commercial codes, like Fluent, are based on fully tested and validated flow-solver which is formulated on finite volume method with segregated grids. However, it will be consistent to state that all flow-solver algorithms are problem-dependent. Therefore, a brief understanding of the differences in their implementation can facilitate the choice of flow-solver for any engineering problem.

1.1.1 Radiative Heat Transfer in Vertical Combustor

Different correlation models for the radiative properties, described by emissivity, absorptivity and transmissivity, of the flue gases at the Vertical Combustor of the CANMET Energy Technology Centre have been investigated by Wendt [1]. In his study, which focused on the evaluation and description of the thermal radiation of flue gases and not on the radiative properties of flames, one of the major challenges identified involves the correlation of the total emissivity and absorptivity of the overlapping bands at different spectral frequencies of the flue gas constituents. Zonal method for predicting radiative heat transfer in furnaces was adopted based on the model of Scholand [2]. The one-dimensional model divides the radiation zone into axial zones with constant temperatures, constant partial pressures, and constant optical properties. This implies that the radial variations in temperature and concentration were averaged. The fundamental approach illustrates a basic method of calculating the radiative heat transfer during the past few decades, but it is not capable of simulating the radiative heat transfer in non-homogeneous media with anisotropic scattering [3]. Therefore, the design of a combustor, based on two-dimensional finite volume approach, is proposed for the radiative heat transfer calculation. This radiative heat constitutes a source term of the energy equation and represents a spectrally, spatially and directionally dependent integro-differential equation [4].

Recent procedures of calculating and analyzing the radiative characteristics include forward Monte Carlo method, finite-volume method, and backward Monte Carlo method [3-5]. The latter approach of Shuai et al. [3] offers the highest computational efficiency when solutions of the radiative heat flux are only needed at a certain location or at the specified direction. However, this approach is not relevant for boiler design when the entire radiative heat flux within the radiation zone of combustor is desired. Also, due to the complexity of radiation model, involving full spectral dimensionality and correlations, simulation based on line-by-line finite volume that depend on standard spectroscopic databank requires a large computer resources [6].

1.1.2 Conjugate Heat Transfer in Compact Heat Exchanger

Recently, combined cycles have been proved to offer the most efficient way to generate electricity. With the combustion of gas, the flue gas can directly drive the combined turbine cycle. However, the combustion of coal results in flue gases with ash particles and chemically aggressive slag can quickly damage the turbine vanes, if the turbine is internally combined with the combustor. Since the Vertical Combustor (VC) is designed for different modes of combustion, including the combustion of coal and bitumen, externally run turbine cycle can be integrated with the existing system. Consequently, the proposed design will require advanced high-temperature heat exchanger, for needed energy recovery from flue gases (see Figure 1).

Compact heat exchanger are been in use for many applications, including automobile radiators, air-conditioning evaporators and condensers, electronic cooling devices, recuperators and regenerators, and cryogenic exchangers. Compact surfaces offer high heat recovery advantage due to their lightweight, space-saving features. The basic plate fins for this heat exchangers includes plain rectangular, plain triangular, wavy, offset strip, perforated, louvred, etc. [7].

Conventionally, the heat duty requirement in the design of heat exchangers demands the determination of the Colburn j factor and the Fanning friction f factor as functions of Reynolds number. Different surface configurations depicted in various plate fins, stated above, present different size and shape relationships with varied performances. However, of these many enhanced fin geometries, offset strip fins are widely used, especially for high temperature applications. They offer a high degree of surface compactness, and substantial heat transfer enhancement. This is due to the inherent periodic building and collapsing laminar boundary layers over the uninterrupted channels formed by the fins and their dissipation in the fin wakes [10]. Three effects are three-dimensional and cannot be captured without stable and accurate model. Experimental validated numerical approach proposed in this project is capable of modeling these surfaces with three-dimensional flow-solver.

1.2 Description of the Vertical Combustion Research Facility at CANMET

The Vertical Combustor Research Facility (VCRF) (see Figure 2) is capable of firing pulverised coal and/or natural gas at the rate of up to 0.3 MW and comparable to normal

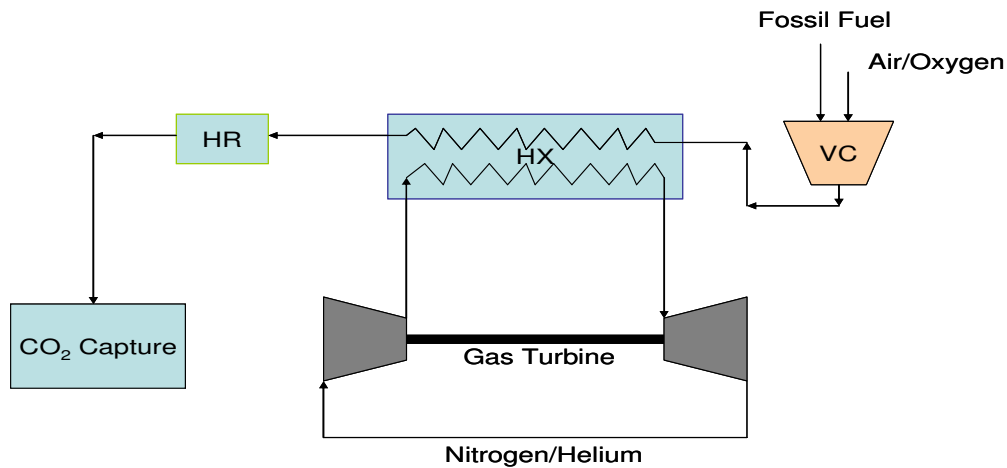


Figure 1 Schematic of the Combined Power Generation Cycle with Nitrogen/Helium as the compressed gas in the heat exchanger

industrial capacity. There are four major systems associated with the VCRF. They are the fuel delivery system, the combustion system, the flue gas treatment system and the instrumentation. The focus of the proposed work is based on radiation characterization in

the combustion system and heat recovery procedure within the flue gas treatment system. However, these four major systems will be briefly described here, but comprehensive report of the four major systems and others can be found in the VCRF documentation [8]. Other subsystems within the VCRF include coal crushing, drying and blending facilities, on-site bulk vessels provided by Air Liquide Canada for the storage of oxygen and carbon dioxide and finally, a gas detection/alarm system for environmental monitoring.

1.2.1 Fuel Delivery System

Crushed and dried coal is fed to a single pulverizer operated in batch mode to prepare approximately 12 hours worth of fuel. Ambient air is used to sweep the mill and entrain the pulverized product to an overhead storage silo. This silo feeds a loss-in-mass-feeder which is capable of maintaining a relatively steady flow of coal to an eductor assembly. Ambient air or carbon dioxide from the bulk storage vessel is used as the primary stream, depending on the experiment, to deliver the coal to the burner front.

1.2.2 Combustion System

The combustion takes place in a vertically down fired combustor that has an inside diameter of 60 cm and an overall length of 8.3 m. The combustor is refractory lined to conserve heat to provide a realistic time-temperature history for the burning particles of coal. The design of the combustor barrel is modular so that sections can be removed or added as needed. Water cooled panels can be inserted in the lower sections to control the outlet flue gas temperature. A variety of access ports are provided along the length of the combustor to facilitate probing, especially within the flame region itself.

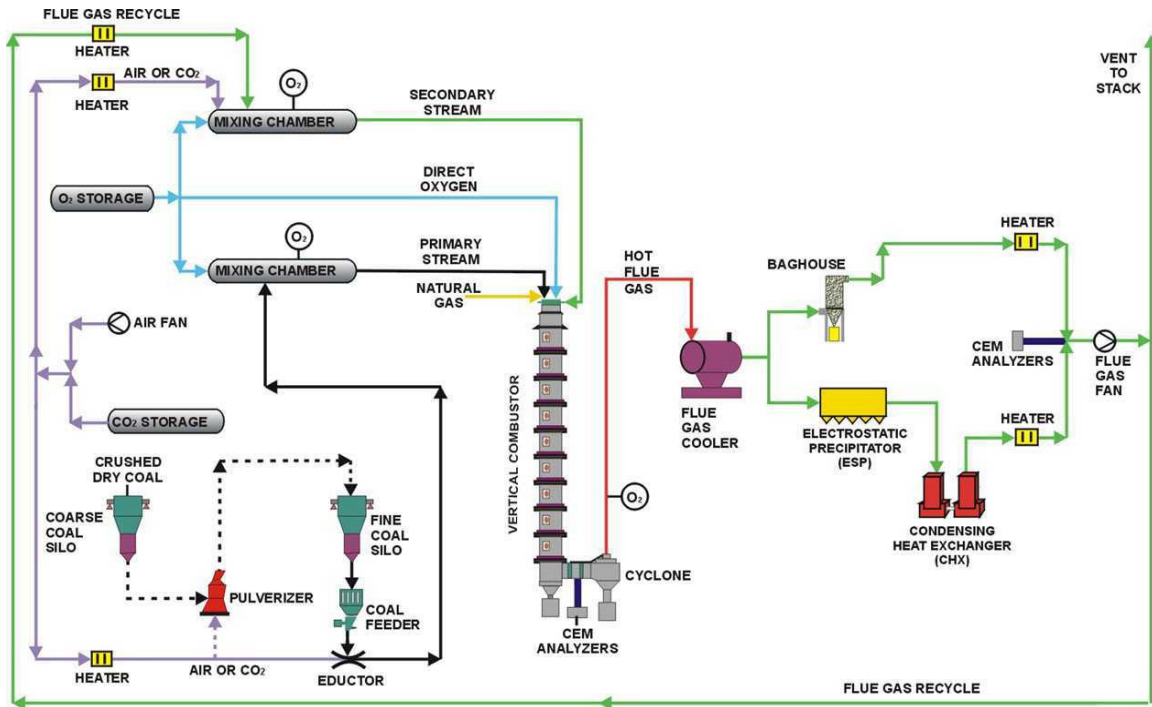


Figure 2 Schematic of the Vertical Combustion Research Facility

1.2.3 Flue Gas Treatment System

Recent modifications have been made to the flue gas system to study the integrated treatment of pollutants. The new equipment is arranged in parallel with the existing baghouse, and consists of a new five field electrostatic precipitator (ESP) and a Condensing Heat Exchanger[®] (CHX). The CHX was made available to CANMET in mid 2000 by McDermott Technologies Inc, and is similar to a unit located in their Alliance, Ohio research center. The CHX unit features Teflon coated gas side surfaces and is configured to inject liquid sorbents over the tubes to capture gaseous pollutants such as sulphur dioxide. The ESP is a custom designed unit supplied by McGill Airclean Corporation in January 2001. It features active control of two field groupings which will facilitate on-line optimization for fine particulate capture.

The flue gas recirculation system has recently been modified to eliminate bottlenecks limiting the throughput and to simplify the fan arrangement. The dedicated recirculation fan has been eliminated and the flue gas recirculation stream is now taken from downstream of the induced draft (ID) fan. The ID fan now operates against a control valve to generate the pressure required by the recirculation system. The ID fan has also been provided with a variable frequency drive for better control.

1.2.4 Instrumentation and Controls

The main burner fires into a refractory quarl which incorporates a natural gas fired ignitor. This ignitor is monitored using an ultraviolet scanner. The coal flame is

monitored using an infrared scanner. The VCRF is provided with three Continuous Emissions Monitoring (CEM) systems to monitor conditions at the mixing plenum before the burner, the combustor exit and the ID fan inlet. Species measured include O₂, CO, CO₂, SO₂, NO and NO₂. An in-situ oxygen cell is used to ensure the oxygen content of the secondary stream is kept below 28 % (dry volume basis) for safety reasons.

As stated, the focus of this work is the modeling of radiative heat flux within the radiation zone of the combustion chamber and the design of compact heat exchanger for heat recovery from the flue gas. A finite volume simulation approach, developed by Energhx Consulting, will be integrated into the solution application.

1.3 Implementation Strategies

The modeling of both the radiative heat transfer characteristics of the VC and the compact heat exchanger design can be formulated with the control volume finite volume method. However, the development of this numerical algorithm is extensive and far beyond the scope of these projects. Computational analysis at this level is normally based on the use of commercial codes, for example FLUENT, CFX and TACSFLOW, etc. These resources are not available for these projects, although initial efforts were made to get a license within the group or seek collaboration with the CFD group. In order to proceed with the required tasks, the use of PlainFlow[®] (a 2-D flow-solver, developed by the President, Energhx Consulting who is also the Visiting Researcher) was proposed. The model will be evaluated and integrated into the application development cycle of the numerical tool for possible solution of the engineering problems.

The modeling of the radiative heat in the VC includes the interactions between radiation and turbulence within the fully-correlated spectral absorption coefficient-temperature of the radiative gas, spectral intensity and the spectral blackbody intensity (or Planck function). Also, the module of activities to be carried out toward the thermo-mechanical design of high-temperature heat exchanger represents the core element for the above cycles. The three major activities involved in this design include the material selection, thermo-fluid design, and the thermo-structural design. Apart from the update of the challenges involved with coupling the highly pressurized process stream with the flue gas stream operating at atmospheric condition, the report includes vital components relating to the software development for the project and the results of activities towards the selection of the materials for the compact heat exchanger. A user-friendly interface for control and monitoring of the system will also be developed using the Microsoft Visual Developing Studio.

2. TECHNICAL PROCEDURES AND MODELLING

Numerical formulation of thermofluid engineering problems involves the solution of the governing equations over a specified solution domain, and subject to well-defined boundary conditions. While the governing equations for most of these problems are typical, the boundary conditions and their treatment are basically varied, depending on the problem formulation. This formulation starts with the discretization of the governing equations, generally known as Navier-Stokes equations. The terms included in the Navier-Stokes equations are the transient term, advection term, diffusion term and the source term (the specific definition of these terms may depend on the problem involved). For example, the natural convective flows has an implicit source term from buoyancy effect; while channel flow problems does not have implicit source term unless if explicitly generated by problem formulation.

Two formulation methods were reviewed, including the Control Volume Finite Element Method (CVFEM) and the staggered grid Finite Volume Method (FVM). One other method of formulating numerical fluid problems is the Finite Difference Method (FDM). The implementation procedure for these methods involves the discretization of the governing partial differential equations, in order to obtain sets of linearized algebraic equations. The algebraic equations describing the system are obtained through balances of the conserved quantities (e.g., mass, energy, and momentum).

2.1 Governing Equations

Generic governing equations for an incompressible fluid, known as Navier-Stokes equations, are as follows:

$$\frac{\partial(\rho_i)}{\partial t} + \nabla \cdot (\rho_i u_i) = 0 \quad (2.1)$$

$$\frac{\partial(\rho_i u_i)}{\partial t} + \nabla \cdot (\rho_i v_i u_i) = -\frac{\partial p_i}{\partial x} + \nabla \cdot (\mu_i \nabla u_i) \quad (2.2)$$

$$\frac{\partial(\rho_i v_i)}{\partial t} + \nabla \cdot (\rho_i v_i v_i) = -\frac{\partial p_i}{\partial y} + \nabla \cdot (\mu_i \nabla v_i) \quad (2.3)$$

$$\frac{\partial(\rho_i c_{p_i})}{\partial t} + \nabla \cdot (u_i T_i) = \nabla \cdot (k_i \nabla T_i) \quad (2.4)$$

However, the specific formulations for each of the problem tasks are formulated according to the changes in the pattern of flow, boundary and initial conditions.

2.1.1 Governing Equations for the Radiative Heat Transfer Problem

Assuming the mixture of the flue gases (i.e., CO₂ and H₂O) and gray particles is modeled with a radially symmetric combustor, the radiative transfer equation (RTE) after integration over the kth gray band, can be written as

$$\frac{dI_k}{ds} = -(\kappa_{g,k} + \kappa_p + \sigma_p)I_k + \kappa_{g,k}\omega_{g,k}I_{b,g} + \kappa_{p,k}\omega_{p,k}I_{b,p} + R_k \quad (2.5)$$

where $\omega_{g,k}$ and $\omega_{p,k}$ are the weighting factor for gas and particles, respectively.

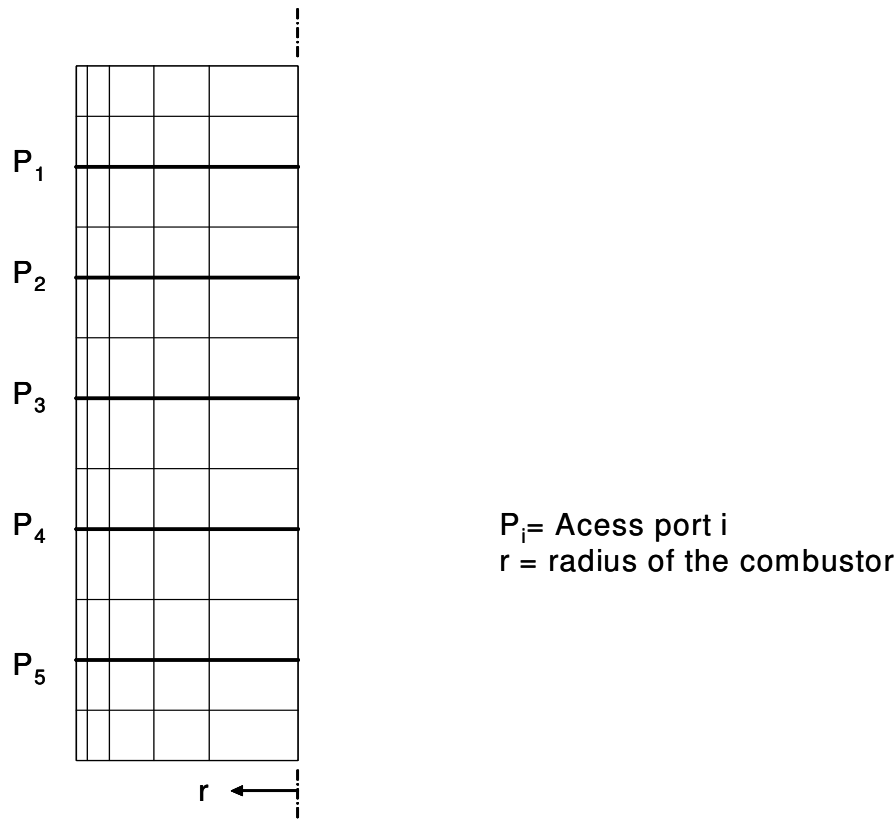


Figure 3 Two-dimensional grid for the Vertical Combustor

The narrow band modified WSGG model based on k-correlated distribution will be adopted for the evaluation of the radiative properties. Using the input data, obtained from the experimental test runs through the five access ports (see Figure 3), different interpolation and extrapolation procedures will be utilized in order to obtain the local variables of all the nodes in the computational domain. Following the Kim and Song's

WSGG model [9], the absorption coefficient is determined for the partial pressure and temperature of flue gases as follows:

$$\kappa_i = \kappa_i^0 \frac{P}{T^2} e^{-\alpha_i / T} \quad (2.6)$$

A two-dimensional control volume finite volume formulation is proposed to solve the RTE in Eqn. (2.5). However, the modeling activities is herefrom discontinued, while the group's mandate is shifted to the design of a compact heat exchanger for the proposed integrated gas-turbine power generation cycle.

2.1.2 Governing Equations for the Heat Exchanger Problem

In addition to the equations given above (Eqns 2.1-2.4) for the fluid system within the heat exchanger, the energy equation of the solid can be written as

$$\frac{\partial(\rho_s c_{ps})}{\partial t} + \nabla \cdot (k_s \nabla T_s) = 0 \quad (2.7)$$

The balance of entropy for a control volume can be written as

$$\frac{\partial(\rho s)}{\partial t} + \nabla \cdot (\rho v s) = -\nabla \cdot \left(\frac{q}{T} \right) + \dot{\mathcal{P}}_s''' \quad (2.8)$$

where $\dot{\mathcal{P}}_s'''$ refers to the entropy production rate (per unit volume) which is solved explicitly from the predicted field variables. Coupled conjugate wall boundary conditions [10], i.e.,

$$T_s = T_i \quad (2.9)$$

$$-k_s \left(\frac{\partial T_s}{\partial n} \right) = -k_i \left(\frac{\partial T_i}{\partial n} \right) \quad (2.10)$$

are imposed at the solid-fluid interface. All other wall surfaces are treated as adiabatic.

2.2 Materials for the Compact Heat Exchanger

The material selection criteria that drive the development of compact heat exchanger are the need for lightweight, space saving, and economical heat exchangers. Compact heat exchangers are characterized by extended surfaces with large surface area/volume ratios, arranged in form of either plate fin or tube fin. The plate fin configuration finds diverse

applications, where the fins have varied surfaces like: plain fins, wavy fins, strip fins and perforated fins. Amongst all, offset strip fins are widely used because they have a high degree of surface compactness [19]. These fins are designed to act as secondary heat transfer surface and also to contain the pressure differential between the streams.

Apart from the design criteria presented above, plate-type compact heat exchangers have found its usefulness in high-temperature applications. Some of these applications which include the combustion of pulverized coal results in flue gases. Coupled with the compressed gas as secondary fluid, the high pressure and the corrosion effects demand a comprehensive thermo-mechanical design for a durable and efficient heat exchanger.

A compact version of heat exchanger made with the carbon-carbon composites is depicted in Figure 4. With an alternative design in the use of molten salt and helium as working fluids, the cross-sectional area of the fins and the thickness of the remaining plate below the machined channels would be adjusted to provide sufficient strength to resist thermal and mechanical stresses.

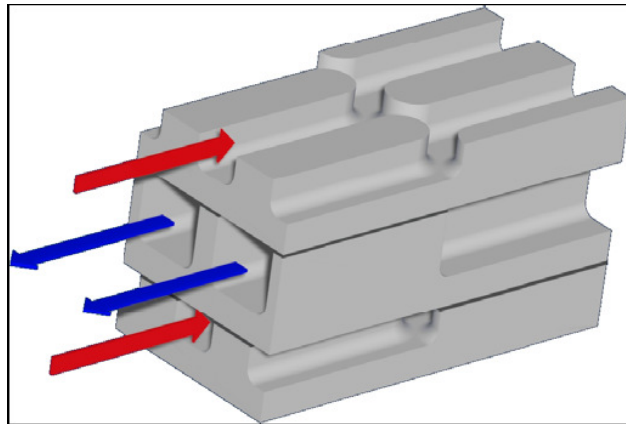


Figure 4 Cut-away plate section of LSI-HX showing alternating molten salt at the inner channels and helium at the outer channels (Source: C.W. Forsberg et al, 2004 [11])

2.2.1 Criteria for Material Selection

Considering the complexity of satisfying the material demands of high-temperature heat exchangers, for use in a vertical combustor which is subjected to varied mode of combustion, a separation of function had to be applied by using an environmental barrier coating (EBC) that ensures the corrosion stability. This selection focuses on the thermo-mechanical stability of the material and the gas impermeability. Suitable materials under consideration for this application include Nimonic PK33 [12], Reaction Bonded SiC [13] and Calcined Alumina [14]. The criteria for selection will include, but not limited to, low coefficient of thermal expansion CTE , low Young's modulus E , high thermal

conductivity k , durability and cost. Available properties of these materials are shown in Table 1.

Table 1 Comparison of the material properties at elevated temperature

	Nimonic		Al ₂ O ₃	SSiC
	90	PK33		
K [W/m K] (1000°C)	27.9	27.2	6	40
CTE [10 ⁻⁶ K ⁻¹] (960°C)	12.7	10.6	7.5	4.6
E [GPa] (20°C)	204	217	340	410
$\sigma_{b,bend}$ [MPa] (20°C)	1175	1127	300	400
T _{max} [°C]	920	900	1700	1600

2.2.2 Proposed Criteria for EBC Selection

Table 1 above shows a comparison of the material properties of some selected materials proposed for the manufacturing of the plate-fin ceramic heat exchanger. In order to obtain the complete comparison with the selection of a suitable EBC for the operating condition, material testing experiments will be conducted in the laboratory. This effort will enable a proper protection of the designed energy system from substance from oxidation.

3. EXERGETIC DESIGN OF COMPACT HEAT EXCHANGER

The Second Law equation describes the state of irreversibility within the boundaries of energy systems. Due consideration of this law in addition to the First Law can provide better estimate of the quality of available heat energy recoverable via the serving stream of the heat exchanger. These two laws of thermodynamics can be written as [7]:

$$\frac{dE}{dt} = \dot{Q}_o + \sum_{i=1}^n \dot{Q}_i - \dot{W} + \sum_{in} \dot{m}h_t + \sum_{out} \dot{m}h_t \quad (3.1)$$

and

$$\dot{S}_{gen} = \frac{dS}{dt} - \frac{\dot{Q}_o}{T_o} - \sum_{i=1}^n \frac{\dot{Q}_i}{T_i} - \dot{W} + \sum_{in} \dot{m}h_t + \sum_{out} \dot{m}h_t \quad (3.2)$$

By eliminating \dot{Q}_o from Eqns (3.1 & 3.2), the work rate output can be maximized as:

$$\dot{W} = -\frac{d}{dt} [E - T_o S] + \sum_{i=1}^n \left(1 - \frac{T_o}{T_i}\right) \dot{Q}_i + \sum_{in} \dot{m}(h_t - T_o s) - \sum_{out} \dot{m}(h_t - T_o s) - T_o \dot{S}_{gen} \quad (3.3)$$

Since \dot{S}_{gen} cannot be negative, the maximum possible work from the system is obtained at the minimum value of $T_o \dot{S}_{gen}$, known as the lost available work or Gouy-Stodola theorem. In order to understand the application of this theorem to heat exchanger design, it will be useful to comprehend the process of entropy generation via the interaction of the streams with the walls.

3.1 Entropy Generation in Heat Exchanger

System optimization demands exergy analysis for all energy systems where power or refrigeration effect is operational. In this case and as it applies to heat exchanger design, the First Law which deals with the conservation of energy will not be adequate, in order to capture the heat and work interaction through the conjugate system.

3.1.1 Basic Components of Entropy Generation

From the First Law:

$$\dot{m}dh = q'dx \quad (3.4)$$

And assuming steady state condition with no work and heat loss or gain from the environment, the Second law states that:

$$d\dot{S}_{gen} = \frac{d\dot{Q}}{T \pm \nabla T} + \dot{m}ds \geq 0 \quad \text{for each side,} \quad (3.5)$$

while the \pm sign denotes either the hot or cold stream of the heat exchanger. Now, the canonical entropy relationship states that

$$\frac{dh}{dx} = T \frac{ds}{dx} + \frac{1}{\rho} \frac{dp}{dx} \quad (3.6)$$

Therefore, entropy generation term (after linking Eqns 3.4 - 3.6) is

$$\dot{S}'_{gen} = \frac{dS_{gen}}{dx} = \frac{q'\Delta T}{T^2(1+\tau)} + \frac{\dot{m}}{\rho T} \left(-\frac{dp}{dx} \right) \quad (3.7)$$

where $\tau = \Delta T / T$, the dimensionless temperature difference. This equation reveals that the two basic components of entropy generation, including the temperature gradient term and the pressure gradient term. Since the heat transfer gradient is directly proportional to the temperature gradient, it implies that the entropy generation rate for the thermal component is proportional to the square of the dimensionless temperature difference τ , and this term plays a vital role in the minimization of the generation of entropy within the energy system.

3.1.2 Minimization of Entropy Generation

Figure 5 reveals the temperature profile for a typical counterflow heat exchanger. Writing Eqn 3.7 in a differential form,

$$d\dot{S}_{gen} = -\left(\frac{q'dx}{T(T+\Delta T)} \right)_p + \left(\frac{q'dx}{T(T+\Delta T)} \right)_s - \dot{m}_p R_p \frac{dp_p}{p_p} - \dot{m}_s R_s \frac{dp_s}{p_s} \quad (3.8)$$

Fictional entropy generation due to pressure drop for liquids (and for limiting perfect gas flow assumption) is negligible, due to the high density in the last two terms in Eqn 3.8. Simplified analysis, with this assumption of zero pressure drops, has adopted two approaches including the balanced counterflow [15] and the flow imbalance [16] procedures. However, the design of compact heat exchanger with imbalanced streams and with possible differential pressure ratios cannot be analysed based on this assumption.

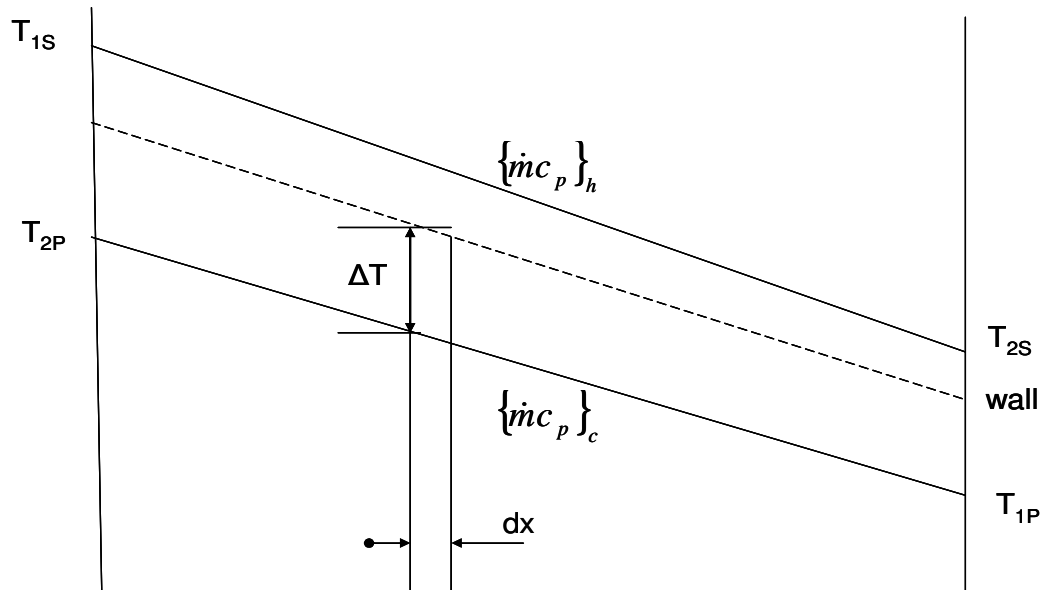


Figure 5 Temperature Profile for Counterflow Heat Exchanger

Substantial correlations for the heat transfer and pressure drop in offset strip fin heat exchanger (see Figure 6) are available in the literature [17]. Although, many of these efforts are dominated by experimental investigation [18], analytical models and numerical solutions [19] have also been developed. Despite the preceding investigative efforts, the prediction of the heat transfer and pressure drop along the channels of offset strip fin heat exchanger remains difficult, and grossly oversimplified. Considering the broad application of offset strip fin heat exchanger, reliable prediction of heat transfer and friction factors is necessary.

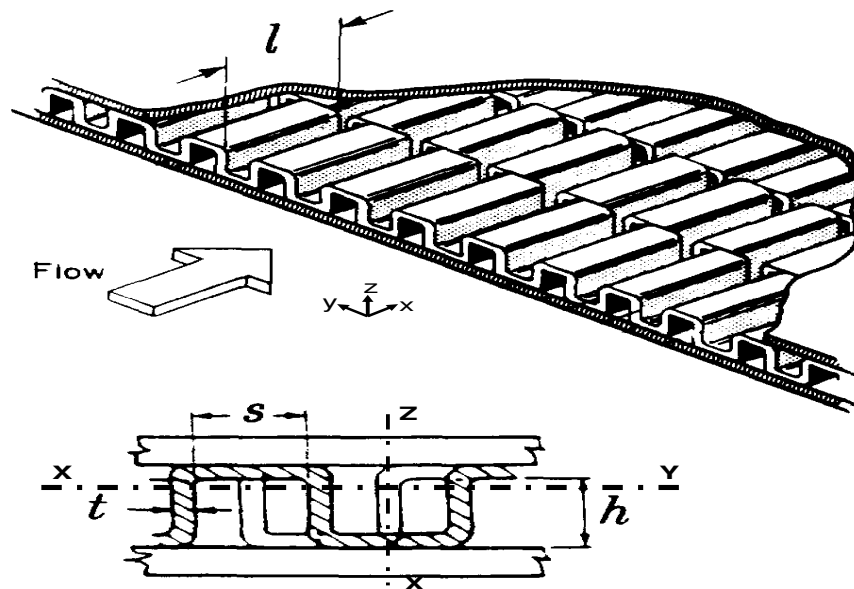


Figure 6 Description of the Offset Strip Fin Arrangement

Apart from the geometry of the fins, the thermal properties of the flue gas can play a significant role in the heat transfer and pressure drop characteristics. The effect of flue gas radiation on the performance of a compact ceramic heat exchanger has been reported by Chen et al [20]. It was reported in their numerical study that, the predicted Nusselt number with surface and gaseous radiation heat transfer was averagely higher than the Nusselt number without radiation heat transfer by 7%. Similar trend was observed for the friction factor comparisons, while the increment in this case was 5%.

3.2 Numerical Approach in Heat Exchanger Design

3.2.1 Thermo-fluid Design

Figure 7 shows the computational domain from section X-Y of the heat exchanger. Navier stokes equations, comprising the conversion of mass, momentum and energy will be used for Nusselt number and pressure drop calculations. The discrete transfer radiation model will be incorporated into the numerical model for radiation calculation.

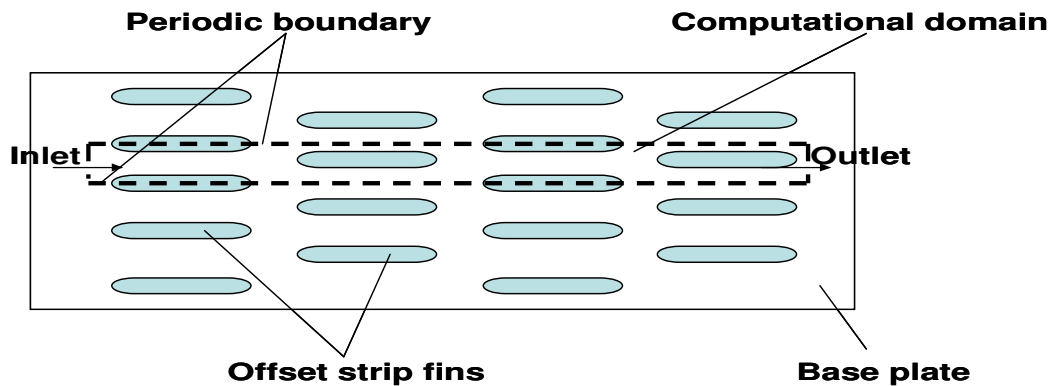


Figure 7 Section X-Y showing the 2-D computational domain for thermo-fluid modeling

The ceramic heat exchanger will be designed based on counter flow configuration and analyzed using LMTD-method.

3.2.2 Thermo-structural Design

Thermo-structural analysis of the heat exchanger represents a significant aspect of the design because of the brittleness of the ceramic materials. This analysis will investigate the stress distribution of the base element and the core section at the operating condition. The predicted temperature distribution for the flue gas and the process gas will be used as the boundary condition.

Figure 8 shows the computational domain from section X-Z of the heat exchanger. Three dimensional finite element modeling of the structure, including the base plate and the offset strip fins, will be carried out.

With different stages of the design implementation as expressed in this and preceding sections, some of these activities involve sub-modules which are omitted in this version of the project plan. However, preliminary milestones detailing the implementation phases will be necessary for a start.

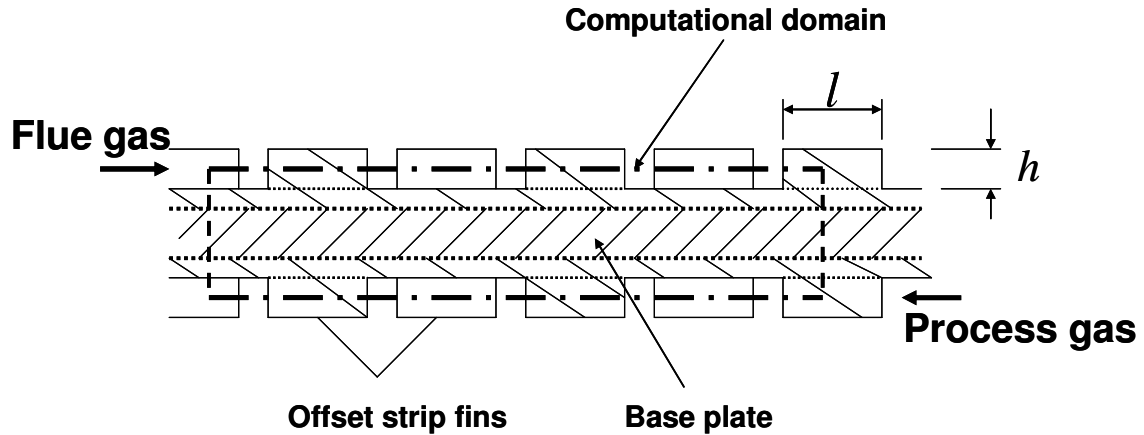


Figure 8 Section X-Z showing the 2-D computational domain for thermo-structural modeling

4. SOFTWARE DEVELOPMENT

The design procedure involves the development and use of extensive numerical schemes based on finite element and volume methods. These schemes represent the flow-solver for the sets of governing equations that describe the flows through the primary and secondary channels of the heat exchanger. Also, the flow-solver is responsible for solving the transport of heat throughout the entire conjugate domain (primary stream, secondary stream, and the core). Apart from description of modules constituting the flow-solver, this chapter discusses the generation of the conjugate domain and the development of graphic user-interface. The documentation of the visualization project is also included in this chapter. These schemes and modules will be used to develop the proposed user-friendly numerical tool for the design of compact heat exchanger. This section highlights issues relating to the development procedure of the use of the proposed code.

4.1 Existing Finite Element/Volume Modules

The numerical solution of the equations governing the transport of fluid flows and heat transfer represents a well-developed field of study, known as Computational Fluid Dynamics (CFD). Two major existing methods which have been used consistently are well-tested and judged as accurate procedures in CFD. These procedures include both the Finite Element Method (FEM) and Finite Volume Method (FVM). The NSERC Post-doctoral Researcher has developed both schemes during his doctoral training at the University of Manitoba. The three-dimensional FEM approach represents the focus of his thesis, where he developed a novel advection scheme, known as the “Non-Inverted Skew Upwind Scheme (NISUS)”[21]. The FVM modules, based on the well-known SIMPLEC approach, were developed in both 2-D and 3-D by him as an extra-thesis curriculum. These methods have been packaged and registered as EnerghxFlow[®] and PlainFlow[®] under the enterprise of the researcher’s Energhx Consulting.

These modules will be used to develop a user-friendly solution for the compact heat exchanger design. These routines have been well-validated and used with the other research interest of the researcher, in the area of microfluidics with the application of second law analysis of slip flow irreversibilities [22, 23, 24, 25]. Present advances (in collaboration with Prof. G.F. Naterer and Prof. M.A. Rosen) in this area of research involves the influence of axial conduction of temperature gradient on slip flow irreversibility in both counterflow-heated and parallel-flow heated microchannels [26, 27].

The following list introduces the basic modules that comprise the PlainFlow[®], which has been used to demonstrate the possibility of using the flow-solver, from Energhx Consulting for the development of the Window-Based Application:

- **Props()** – This module calculates the point mass and diffusivity of the domain.
- **Massp()** – This module calculates the cell-interface mass-flowrates at P.
- **Massu()** – This module calculates the mass-flowrates on the u-control volumes.
- **Massv()** – This module calculates the mass-flowrates on the v-control volumes.
- **Difu()** – This module calculates the diffusion coefficients for the u-control volumes.
- **Difv()** – This module calculates the diffusion coefficients for the v-control volumes.
- **Weight()** – This module calculates the convective and diffusive weights on the coefficients of the momentum and scalar transport equations.
- **Coeff()** – This module calculates the coefficients of all transport equations.
- **Sorcu**() – This module calculates the source term in the u-momentum equation.
- **Sorcv**() – This module calculates the source term in the v-momentum equation.
- **Bndcu**() – This module insert the boundary conditions for the u-momentum equation.
- **Bndcv**() – This module insert the boundary conditions for the v-momentum equation.
- **Bndct**() – This module insert the boundary conditions for the energy (temperature) equation.
- **Bcelim()** – This module modifies the boundary coefficients in order to incorporate fictitious boundary specifications.
- **Chat()** – This module asserts modifiers for the pressure equation.
- **Coefp()** – This module calculates the coefficients for the pressure equation.
- **Sorcpu**() – This module calculates the source term for the u-p coupling.
- **Sorcpv**() – This module calculates the source term for the v-p coupling.
- **Lgs2d()** – This module represents the iterative solver, based on Tri-Diagonal Matrix Algorithm.
- **Sorcp**() – This module calculates the source term for the pressure equation.
- **Velcor()** – This module corrects/updates the velocity field for the next iteration.
- **Pcor()** – This module corrects/updates the pressure field for the next iteration.
- **Bndcp**() – This module specifies pressure level at the boundary.
- **Difphi**() – This modules calculates the diffusion coefficient for the scalar transport equation.
- **Sorct**() – This module calculates the source term for the scalar transport equation.
- **Prod()** – This module calculates the entropy generation distribution.
- **Resid()** – This module monitors the residual from equation solution at current step.
- **Range()** – This module calculates the range value for the convergence criteria.
- **Heatflow()** – This module calculates the heat transfer across the walls.
- **Presdrop()** – This module calculates the pressure drop across the channel.

4.2 Adaptation of PlainFlow[®] to Project Development

The modules constituting the flow-solver were developed with the native `_cdecl` convention, using the C++ programming language. However, the development studio for the window-based application is the Microsoft Visual 2005, using the CLR Window Application framework. Since this framework develops class-based methods for the graphic user-interface, class wrappers will be required to adapt the previously developed native codes. The design of compact heat exchanger depends on accurate understanding of fluid flow and conjugate heat transfer. This understanding plays a significant effort in the evaluation of PlainFlow[®] within the Microsoft Development Studio.

The two-dimensional method of PlainFlow[®] is necessary for validation of the conjugate modeling of the heat transfer between the two streams through the solid core (see Figure 8). Also, the time-saving advantage of the two-dimensional analysis will provide a shorter design cycle. A single sample case can run for almost two weeks before steady-state convergence. However, the incorporation of the strip-fins within the flow fields will require three-dimensional modeling. This will enable the capturing of effects that are typified in Figure 7 & 8.

The modeling of a conjugate domain, including two separate fluid regions and a solid region, represent the major contribution in this project. This challenge is embodied in the generation of the grids representing the entire domain in such a way that the output can be passed into PlainFlow[®] for computation of the field variables. Two methods are presented, including multi-threading approach and collocated approach. Also, the development of the user-friendly interface involves the use of the Microsoft Visual Studio to design window forms with control boxes. The detail descriptions of these procedures, as shown in Figure 9, are described in the following subsections.

4.2.1 Multi-threading Approach

The multi-threading approach is based on the new .NET framework of the Microsoft Development Studio. The computation of the two flow fields are solved separately but simultaneously, using two threads within the same processing unit. This method can save computation time, shown in Figure 10, as expressed by the Courant number (CFL).

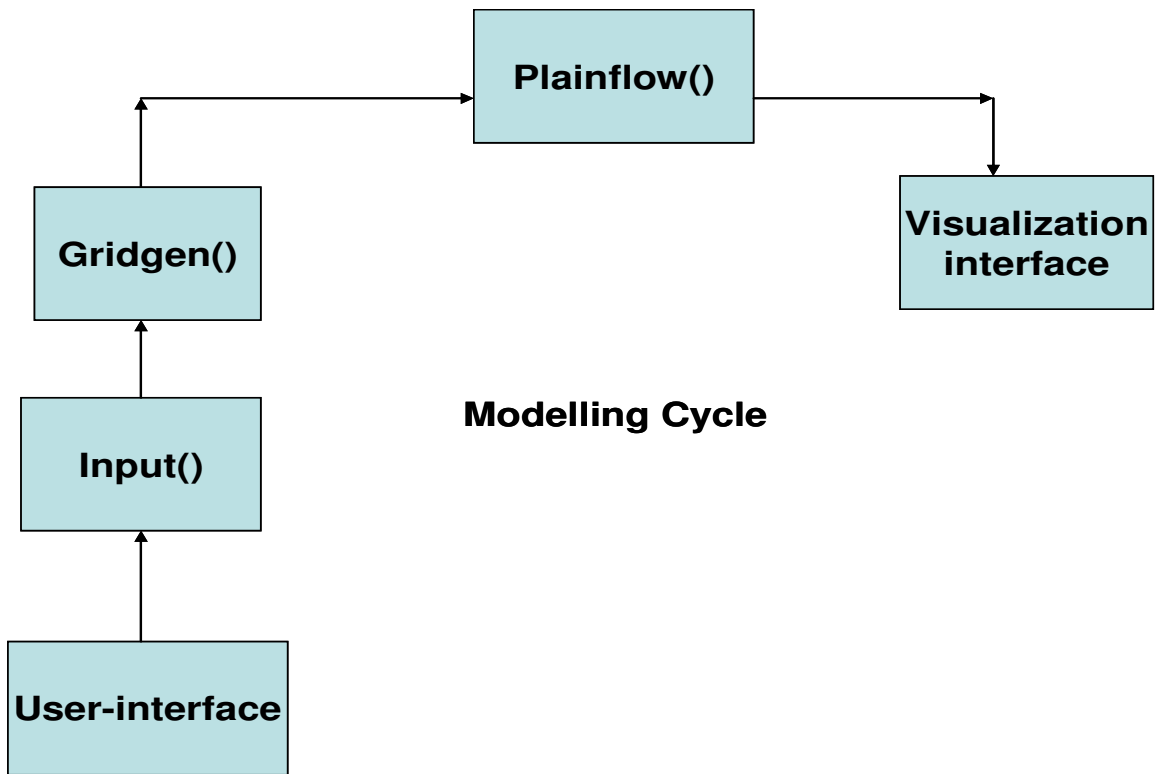
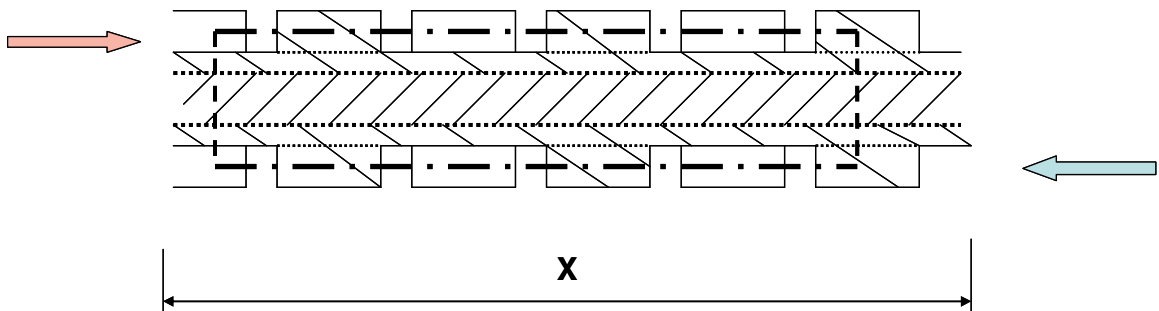


Figure 9 The Software Development Cycle



For unthreaded computation,

$$t = \{(Nx)(CFL)(dx)/v\}_p + \{(Nx)(CFL)(dx)/v\}_s$$

For threaded computation,

$$t = \{(Nx)(CFL)(dx)/v\}_{average}$$

Figure 10 Multi-threading Approach for heat exchanger design

This approach is implemented by developing separate grids for both streams. The output from the grid generator and input parameters are passed into PlainFlow[®] for field calculation of velocities, pressure and temperature. The time-splitting scheme is proposed to be developed to integrate the results of the two streams with the solution of the energy equation for the solid core. One major challenge encountered involves the differential time-matching of one stream under atmospheric condition with the other stream under highly pressurized condition. This problem is solved with the collocated approach, which solves the complete field variables for the conjugate system using a single computational domain.

4.2.2 Collocated Approach

A new collocated gridgen() is developed as a single domain of both the two fluid streams and the solid core. Although, the computational demand of the collocated approach is more than that of the multi-threading approach, it is more stable with the differential time-matching analysis.

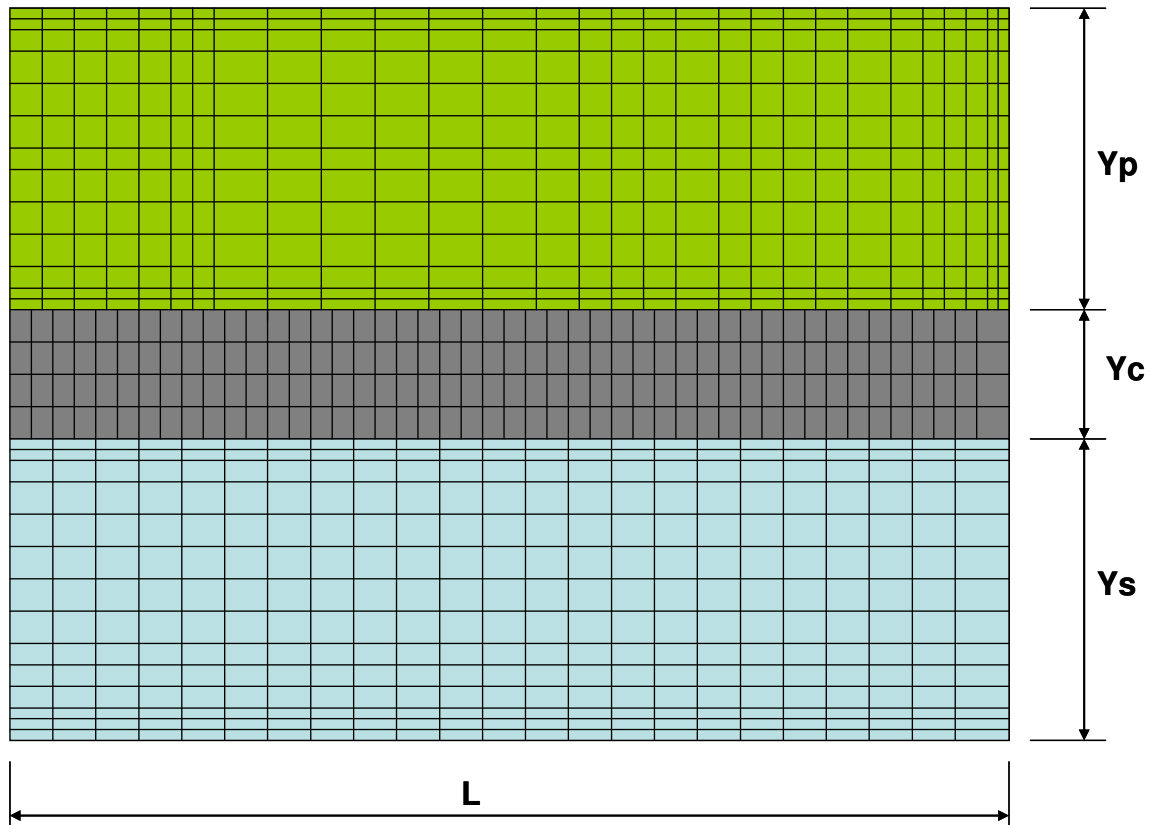


Figure 11 Collocated 2-D Grids for Flow Field Calculation

The differential time-matching between the different grids within the domain is captured by supplying the flow-solver with different matching time-steps. These inputs with others, including the boundary conditions, are linked with the flow-solver using a user-friendly interface.

4.3 Interface Development

Microsoft runtime is the foundation of the .NET Framework. It is responsible for managing code at execution time, providing core services such as memory management and thread management while enforcing code safety and accuracy. Code that targets the runtime is known as managed code while code that does not target the runtime, as is the case with PlainFlow[®], is known as unmanaged, or native code. This framework allows the incorporation of dynamic link library like PlainFlow[®] and other subroutines, including gridgen() and input().

A rich Windows user interface (see Figure 12) for the input and boundary condition parameters is constructed using a subset of `System.Windows.Forms` and `System.Drawing` classes. The implementation of Windows Forms under the .NET Framework includes support for

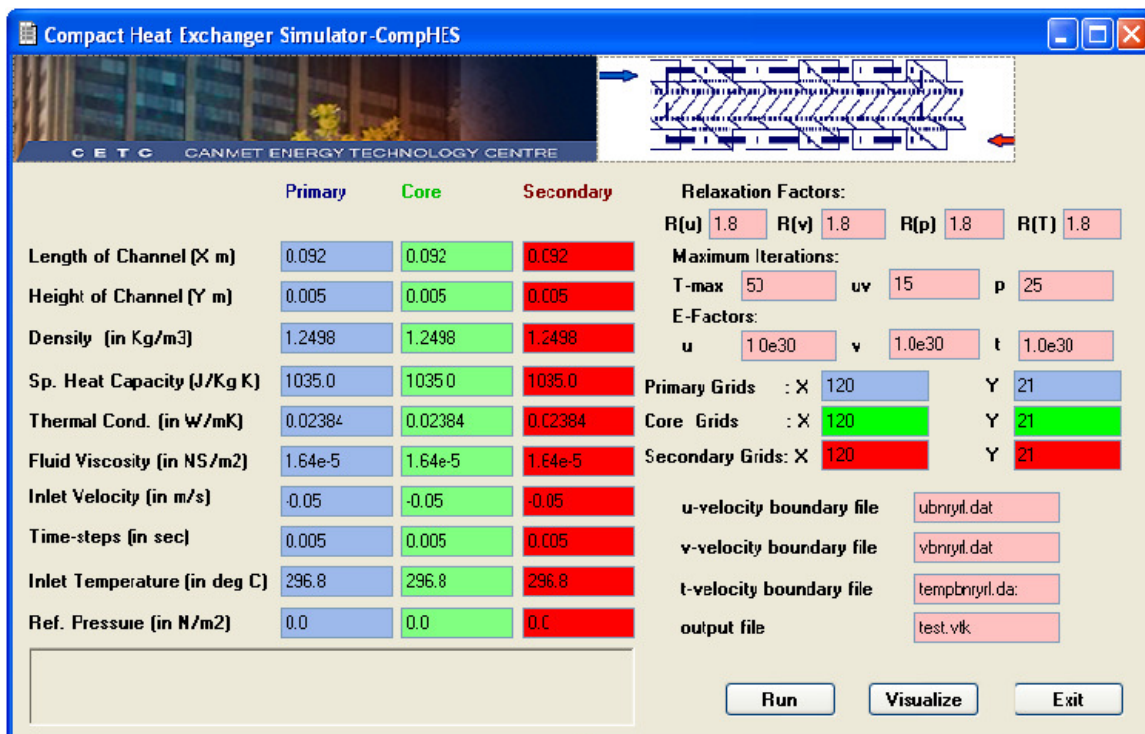


Figure 12 Graphical User-Interface for the Heat Exchanger Simulator

forms, most controls found in the .NET Framework, bitmaps and menus. Table 2 lists the controls included in the design of the user-interface.

Table 2 Controls included with the .NET Framework

Control	Description
Button	simple command button
CheckBox	common checkbox

Label	simple control for displaying text
PictureBox	display images
TextBox	standard text input field

Apart from the thermo-physical properties of the domain described on the Windows Forms, the target files for the boundary conditions to be applied are provided. A general approach adopted in PlainFlow[®] recognize different boundary conditions through some combination of h_{∞} , T_{∞} , and q''_{spec} . Depending on the boundary condition prescribed, the different sides of the conjugate are adjusted accordingly. For example, the boundary conditions on the inlet and outlet primary stream side of the domain are as follows:

Dirichlet temperature at the inlet:

$$T_L = T_{spec}$$

Neumann temperature at the outlet:

$$q''_L = q''_{spec}$$

A typical generalized boundary condition parameter in the boundary files are implemented as summarized below:

Table 3 General Boundary Condition Parameter

Boundary Condition Type	h_{∞}	T_{∞}	q''_{spec}
Dirichlet	10^{20}	T_{spec}	0
Neumann	0	0	q''_{spec}

It is proposed that this interface will be linked also with the visualization API, which will display the results of the simulation at completion and also monitor the progress at runtime.

4.4 Visualization Project

Visualization is a technique used to communicate messages using images, diagram plots and animations. Apart from the scalar data generated by `gridgen()`, the computed field variables (velocities, pressure and temperature, entropy, etc) are predictions which can be presented in form of visual graphics. Scientific visualization is usually done with specialized software, though there are a few exceptions. Some of these specialized programs have been released as open source software, with models and frameworks for building visualizations popularized by systems such as AVS, IRIS Explorer, and VTK toolkit. The latter is proposed to be linked with the user-interface described in section 6.4.

The graphics model in VTK is at a higher level of abstraction than rendering libraries like OpenGL or PEX. This means it is much easier to create useful graphics and visualization applications. The VTK source code is written in C++, so it is easy to be deployed with present application projects whose components have all been written directly in C++. Using the interpreted languages like Tcl or Python with Tk, and even Java with its GUI class libraries, it is possible to build useful applications. However, it is possible to interact with the entire coding framework, including flow-solver, graphic interface, and the visualization pipeline within the Microsoft Visual Studio in C++ without a need for language interpretation.

Visualization pipeline starts with the reading of CFD results from a formatted data file. VTK provides a number of source and writer objects to read and write popular data file formats. The legacy formats are serial formats that are easy to read and write either by hand or programmatically. However, these formats are less flexible than the XML based file formats that support random access, parallel I/O, and portable data compression [28]. For simplicity, the legacy file format is adopted in this project.

4.4.1 Legacy Data Format

The legacy VTK file formats consist of five basic parts, as listed below:

- The first part is the file version and identifier. This part contains the single line: # vtk DataFile Version 5.0. This line must be exactly as shown with the exception of the version number x.x, which will vary with different releases of VTK.
- The second part is the header. The header consists of a character string terminated by end-of-line character \n. The header is 256 characters maximum. The header can be used to describe the data and include any other pertinent information.
- The next part is the file format. The file format describes the type of file, either ASCII or binary. On this line the single word ASCII or BINARY must appear.
- The fourth part is the dataset structure. The geometry part describes the geometry and topology of the dataset. This part begins with a line containing the keyword DATASET followed by a keyword describing the type of dataset. Then, depending upon the type of dataset, other keyword/data combinations define the actual data.
- The final part describes the dataset attributes. This part begins with the keywords POINT_DATA or CELL_DATA, followed by an integer number specifying the number of points or cells, respectively. (It doesn't matter whether POINT_DATA or CELL_DATA comes first.) Other keyword/data combinations then define the actual dataset attribute values (i.e., scalars, vectors, tensors, normals, texture coordinates, or field data).

For the Unstructuredgrid dataset used in this project, the legacy data format can be illustrated as follows:

```
DATASET UNSTRUCTURED_GRID
POINTS n dataType
```

```

p0x p0y p0z
p1x p1y p1z
...
p(n-1)x p(n-1)y p(n-1)z
CELLS n size
numPoints0, i, j, k, l, ...
numPoints1, i, j, k, l, ...
numPoints2, i, j, k, l, ...
...
numPointsn-1, i, j, k, l, ...
Simple Legacy Formats 5
CELL_TYPES n
type0
type1
type2
...
typen-1
FIELD dataName numArrays
arrayName0 numComponents numTuples dataType
f00 f01 ... f0(numComponents-1)
f10 f11 ... f1(numComponents-1)
...
f(numTuples-1)0 f(numTuples-1)1 ... f(numTuples-1)(numComponents-1)
arrayName1 numComponents numTuples dataType
f00 f01 ... f0(numComponents-1)
f10 f11 ... f1(numComponents-1)
...
f(numTuples-1)0 f(numTuples-1)1 ... f(numTuples-1)(numComponents-1)
...
arrayName(numArrays-1) numComponents numTuples dataType
f00 f01 ... f0(numComponents-1)
f10 f11 ... f1(numComponents-1)
...
f(numTuples-1)0 f(numTuples-1)1 ... f(numTuples-1)(numComponents-1)

```

A method known as *vtkLegacyEcho*() is developed to write the legacy file from the CFD code after convergence. This datafile (with extension “vtk”) represents an input into the visualization pipeline.

4.4.2 Visualization Pipeline

The standard rendering classes used in the visualization pipeline (see Figure 13) includes *vtkRenderer*, *vtkRenderWindow*, and *vtkRenderWindowInteractor*. The dataset is read with *vtkUnstructuredGridReader* into the contour filter, known as *vtkGenericContourFilter*. The entire visualization pipeline is developed as a separate CLR class library which can be referenced by the Window Form Application at runtime.

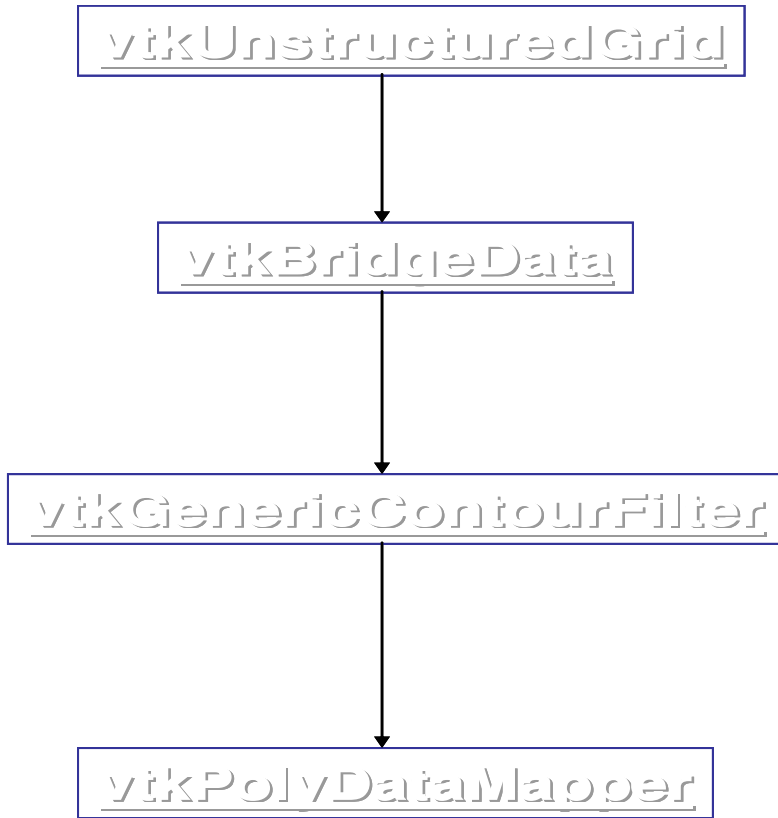


Figure 13 Visualization Pipeline for Contour Plotting

5. RESULTS, DISCUSSIONS AND CONCLUSIONS

Several cases with different flow configuration have been simulated in order to confirm the appropriate mass flow rates for the two-dimensional model. Results for the cases (with $L=1.5\text{m}$, $Y_c=0.015\text{m}$, $Y_p=0.02\text{m}$ and $Y_s=0.05\text{m}$) have been predicted for mass flow rates of $\{6.0\text{ kg/s}, 3.0\text{ kg/s}\}$ and $\{4.0\text{ kg/s}, 2.0\text{ kg/s}\}$ for the primary and secondary streams respectively. Each of the cases reveals a steady state convergence based on the primary stream criteria at the 100,000 iterations. However, the predicted velocity and temperature profiles show that the mass flow rates are too high for these flow configurations. The steady state results maintained a fully developed profile in both streams from the inlet region to the exit region. The latter case converged at 128,765th iteration when the convergence criteria are based on both the primary and secondary streams.

5.1 Results and Discussions

Figure 14 shows the temperature contour for a typical counterflow conjugate wall. Both the process stream and the flue gas stream are simulated with the thermophysical properties of Nitrogen and Air respectively.

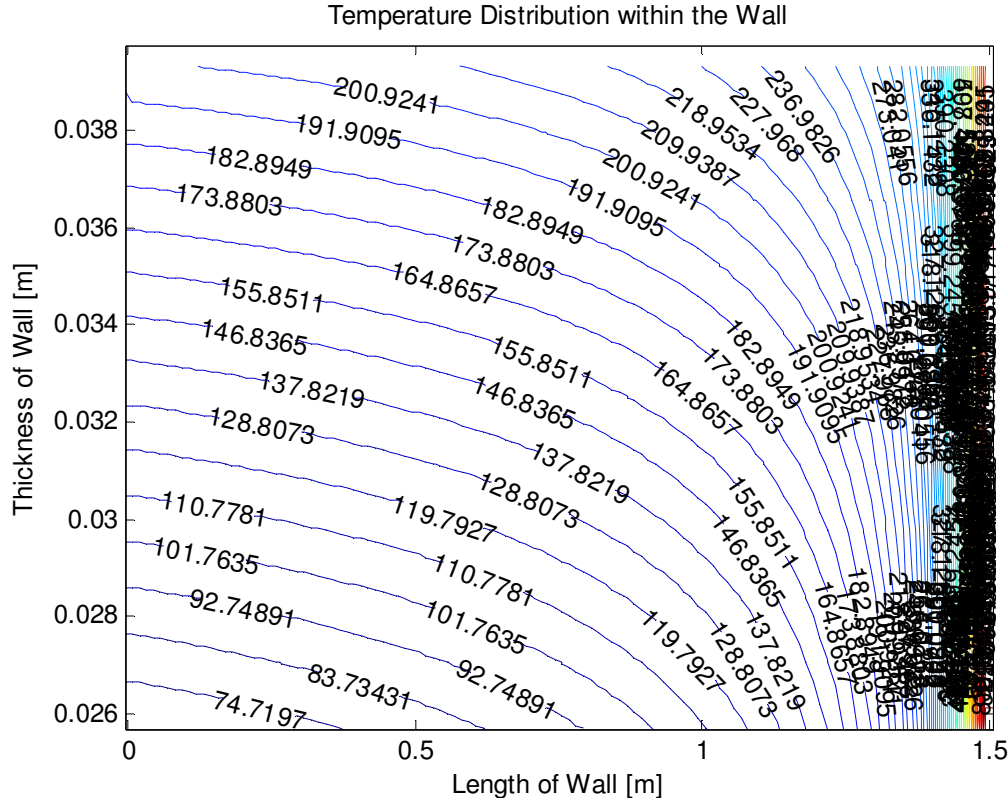


Figure 14 Temperature Contour within the Core

The gradient of heat across the core of the heat exchanger is greatly enhanced with fins arrangement and periodic reattachment of the thermal boundary layer. These effects are omitted in the present simulation because of the two-dimensional limitation. Figure 15 predicts the entropy distribution at $Re \sim 2200$ along the flue gas stream. These distributions follow the pattern of the thermal boundary layer and will play a significant role in the exergetic analysis of the compact heat exchanger.

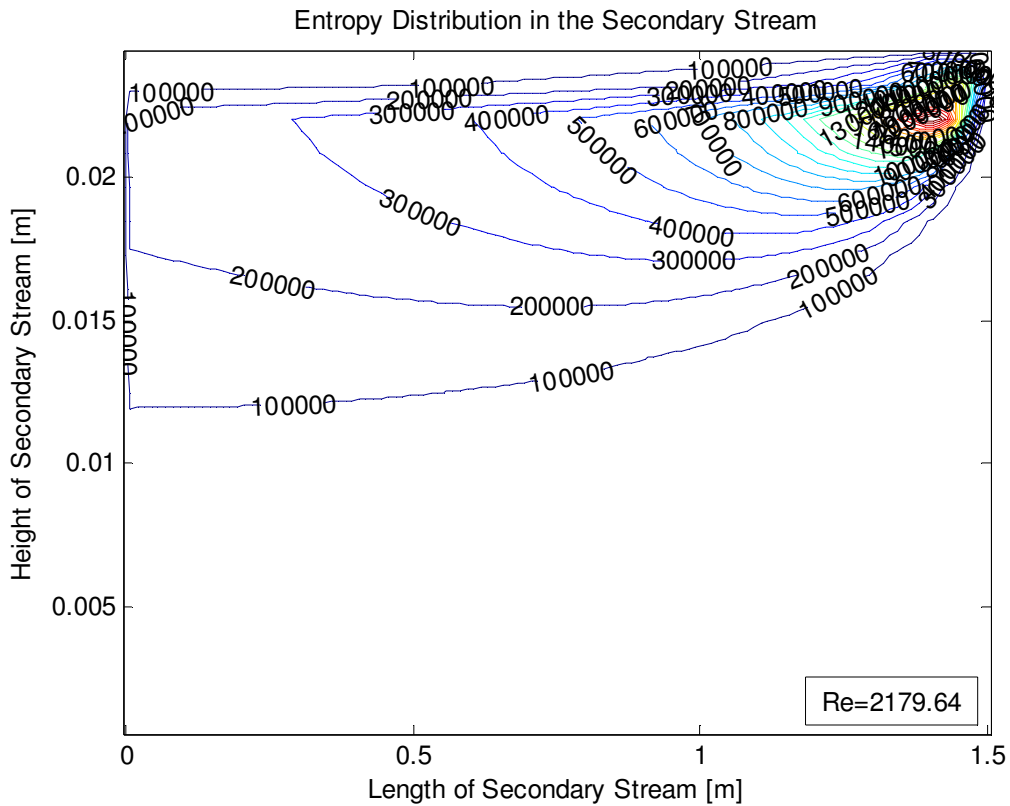


Figure 15 Entropy Distribution Contour along the Flue Gas Stream

5.2 Further Work and Recommendations

The progress report on the modeling of radiation characteristics in the Vertical Combustor and the design of a ceramic high-temperature heat exchanger has been presented. The radiation modeling project is truncated at the literature review and modeling set-up stage, in order to focus on the compact heat exchanger project. Apart from the description of the material selection criteria, the detail implementation procedure for the numerical modeling has been described. The numerical analysis is possible with the evaluation of flow-solver (PlainFlow[®]) from Energhx Consulting. The visualization pipeline is re-modelled (but not fully integrated into the Window Form Application) using an open-source modules provided by Kitware, Inc. Also, the development of the graphical user-interface is possible with Microsoft Visual Studio.

A typical heat transfer profile for the proposed compact heat exchanger has been validated. The history of the Nusselt number across the solid boundary is consistent for a counter-clockwise heat flow arrangement. The entropy distribution with the intermittent development of the thermal and velocity boundary layers due to the proposed offset-strip fins can provide useful design leverage.

On condition of agreement with Energhx Consulting (see Appendix), it is proposed that three-dimensional simulation of the flow-fields including the modeling of the offset-strip fins will be developed using the Energhx 3D Flow-Solver called EnerghxFlow[®]. The revised scheduling of future activities is described in Table 4.

5.2.1 Modelling of the Offset-Strip Fins

The physical model of the compact heat exchanger, as shown in Figure 6, includes the arrangement of the offset-strip fins. The present analysis with two-dimensional model includes the symmetric boundaries at the middle of each fluid stream. With this model, there is no provision for the periodic boundary effects of the fins. The flow pattern in offset-strip finned heat exchanger can be fairly complex due to the three-dimensional nature of the flow separation and helices. The gridgen module will be re-developed in order to facilitate the capturing of both symmetric and periodic boundary conditions. The

The VTK visualization can provide interesting information about the collapsing and re-connecting thermal boundary layer. The proposed toolkit will interact with the new gridgen module before passing data into EnerghxFlow[®] for flow field computation.

5.2.2 Thermo-structural Modelling

Thermo-structural analyses of the ceramic materials for the design of the proposed compact heat exchanger depend strongly on the predicted temperature distribution of the thermo-fluid model. Using the predicted temperature distribution, the behaviour of the composite material under thermal, thermo-chemical and mechanical loads will be studied. With a well-developed model and accurate prediction of thermal loads, a general approach to carry out thermo-structural analysis and how the behaviour is incorporated in the modelling should be straightforward.

5.2.3 Manufacturing of the Prototype

The material selection for the ceramic plate and EBC has been concluded. The manufacturing of the prototype is expected to follow the conclusion of the modeling described in sections 5.2.1 and 5.2.2. This arrangement with possible involvement of other members of the group will be approved by the Group Leader.

Table 4 Scheduling of all the activities involved for the design of ceramic heat exchanger

Activities		Deliverable Target Date											
		Jul-07	Aug-07	Sep-07	Oct-07	Nov-07	Dec-07	Jan-08	Feb-08	Mar-08	Apr-08	May-08	Jun-08
Numerical Modeling	Numerical modeling of the heat transfer and pressure drop												
	Development of interface classes with Visual Studio												
	Numerical modeling of the conjugate heat transfer												
	Development of the visualization interface with VTK												
Design of the Heat Exchanger	Modelling of the fins												
	Analysis by the LMTD or NTU												
Selection of suitable ceramic and binding materials for the manufacturing of high temperature heat exchanger	Characterization of high temperature ceramic materials												
	Experimental testing of the materials, with or without EBC												
Manufacturing of the pilot scale ceramic heat exchanger	Set-up of prototype												
	Testing and collection of data												
	Verification of data with numerical model												

Summarily, it is recommended that:

- The Zero-Emission Technology Group (Group) agrees on the use of PlainFlow[®] and EnerghxFlow[®] from Energhx Consulting. This agreement will enable the integration of three-dimensional modeling of the heat exchanger.
- The Group may purchase additional computer in order to reduce design time, due to debugging of coding activities and testing.
- In case the software agreement is not possible, the original proposal of using commercial code will be inevitable. However, all efforts on graphical user-interface, grid generation and visualization are not portable with commercial software.

- Also, it may be possible to find an open-source CFD code somewhere else. The CFD code does not need to be developed with C++ in order to be portable with the already developed Microsoft Visual Studio platform in this project.

5.3 Conclusions

In conclusion, this report has presented the progress of activities that were undertaken in the group within the period of one-year of research fellowship. These activities include literature review, the material selection, numerical modeling of the conjugate thermofluid system using a two-dimensional model, known as PlainFlow[®] from Energhx Consulting. Also, a user-friendly interface based on Microsoft Visual studio and the visualization projects were developed. The developed models have ascertained that the conjugate discretized model can be incorporated into three-dimensional system where the modeling of the offset-strip fins is possible.

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