INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of HyPEP, A Hydrogen Production Plant Efficiency Calculation Program

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Research Objectives

This research project will evaluate and optimize cycle efficiencies for producing hydrogen and electricity in a Very-High-Temperature Reactor (VHTR). Systems for producing electricity and hydrogen are complex and the calculations associated with optimizing these systems are intensive, involving a large number of operating parameter variations and many different system configurations. This research project will produce the HyPEP computer model, which is specifically designed to be an easy-to-use and fast-running tool for evaluating nuclear hydrogen and electricity production facilities. The HyPEP computer model accommodates flexible system layouts and its cost modeling capability makes it well-suited for system optimization.

Specific activities of this research are designed to develop the HyPEP model into a working tool, including 1) identifying major systems and components for modeling, 2) establishing system operating parameters and calculation scope, 3) establishing the overall calculation scheme, 4) developing component models, 5) developing cost and optimization models, and 6) verifying and validating the computer code. Once the HyPEP code is fully developed and validated, it will be used to execute calculations on candidate system configurations.

Research Progress

The research team began the first task of this project, which includes defining the scope of system modeling in HyPEP by identifying and hierarchically categorizing the major systems, components, and the operating parameters of the Nuclear Hydrogen Development and Demonstration (NHDD) facility and the Next Generation Nuclear Plant (NGNP). During the first three months, they evaluated and selected a programming language, set up the overall model/calculation requirements, and established the hierarchical system/component modeling system. The component hierarchy has been defined and the overview is shown in Figure 1. The results will form the basis of the plant modeling interface of HyPEP and help define the thermal-hydraulic processes and phenomena to consider.

Researchers have begun formulating the numerical solution scheme and established the following overall outline. The node-link-block is the basic fluid/heat flow network scheme:

- Node component handles chemical reactions for the high-temperature electrolysis and thermo-chemical systems. It represents thermal-hydraulic (T/H) volume with scalar properties (e.g., volume, mass, molar fraction, energy, pressure, temperature).
- Link component models flow between nodes and has such properties as mass flow rate, pressure drop, and the scalar properties of the donor-node.
- Block component represents the solid structures that conduct or generate heat and provides models for the solid-to-fluid boundaries where convection occurs.

The basic equations consider the steady-state mass and energy transport of reactive multi-species fluid mixtures. General thermo-dynamic table search routines have been written and are being tested. The routines are developed with options for user-added property tables.

Researchers have evaluated four programming languages: Visual C++, Visual Basic, Fortran, and Delphi. They have tentatively selected Delphi for the HyPEP development. Delphi is an object-oriented version of the PASCAL language and has versions for the .NET as well as the win32 environments. As HyPEP will have a strong

hierarchical structure, the object-oriented program language was deemed to best suit the programming style. The language comparison is summarized in Table 1.

The team initiated development of the base algorithms for the graphical user interface (GUI). They have set up a basic "prototype windows form" to test GUI routines, which is shown in Figure 2. They have also written support routines to enable implementation of the GUI features, which are currently being tested. These routines facilitate on-screen manipulation of components.

Planned Activities

At the end of year 2006, it is expected that a working preliminary version (alpha version) of the HyPEP program will be produced. Major planned R&D activities are as follows:

- **Basic Equation Setup and Numerical Solution Development**. Researchers will set up steady state mass and energy conservation equations for Flow Network. A numerical solution scheme will be developed for flexible network topology. Ancillary routines to obtain T/H properties, heat transfer correlations, pressure drop correlations, etc., will be developed and coded. The numerical scheme will be coded to produce a preliminary working code, and verification and refinement are planned for the next fiscal year.

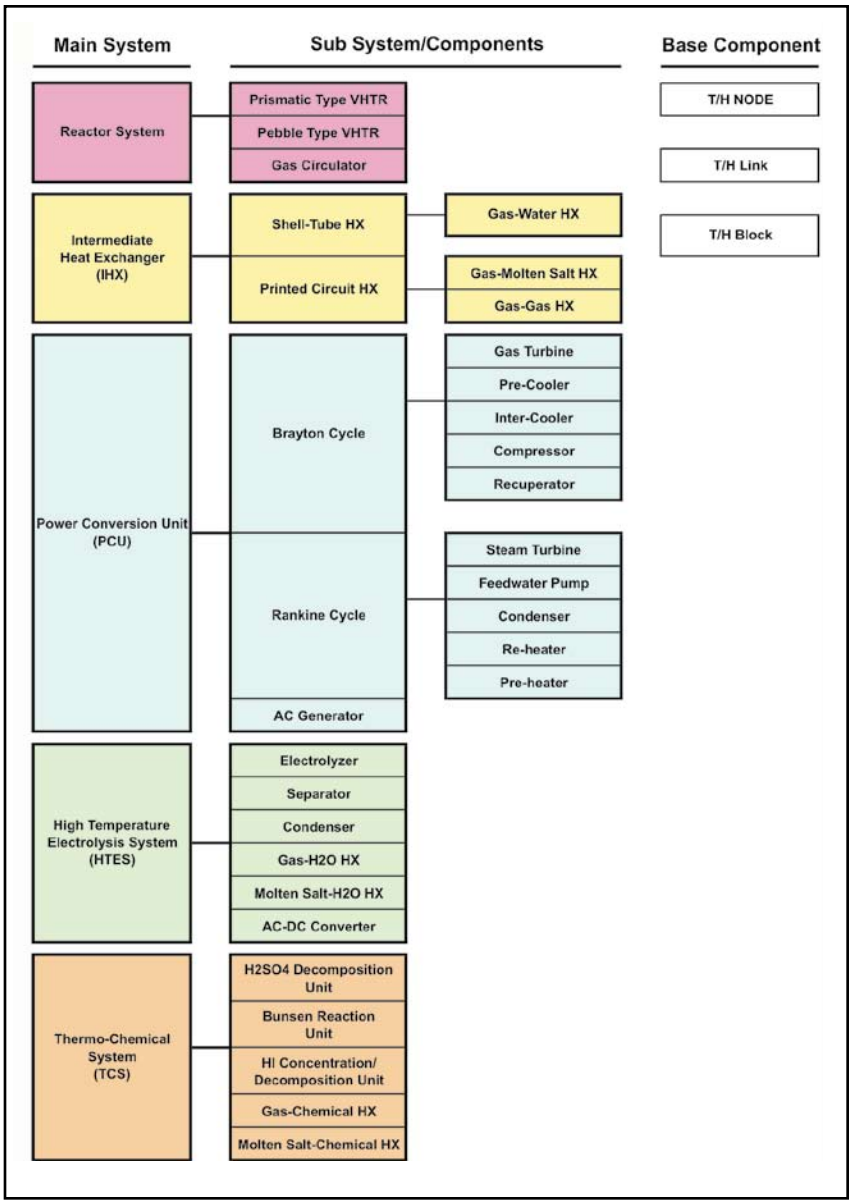

Figure 1. Hierarchical system/component of HyPEP.

Features/Comments	DELPHI	C#	Visual Basic	Fortran
Base Language	Pascal	C	Basic	Fortran
Win32 Version	Delphi2005	C++	MS Visual Basic	Compaq, Lahey etc.
NET Version Common Language Runtime	Delphi2005	MS C# Borland C# etc.	MS Visual Basic	Intel Fortran
OOPS Capability	Very Good	Very Good	Good	No
Structured Programming	Good	Good	Good	Poor
Body of ready-made scientific software	Small	Small	Small	Large
Code Reusability	Good	Good	Fair	Poor
Web Programming Capability	Good (ASPX, ActiveX))	Good	Good (ActiveX)	Poor
Integrated Development Environment	Good	Good	Good	Good
Rapid Application Development (RAD)	Good	Fair	Fair	Poor

Table 1. Comparison of major programming languages.

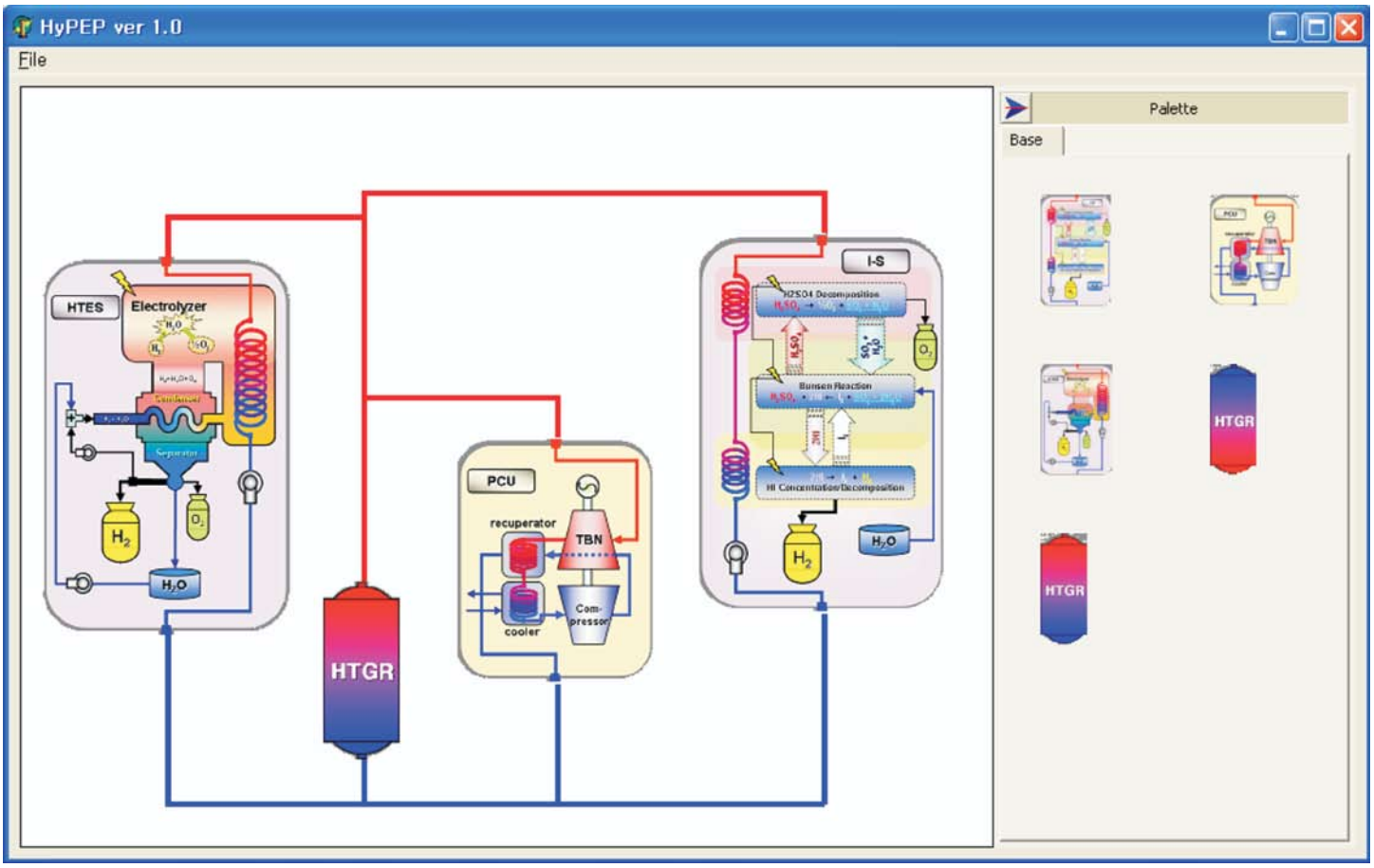

Figure 2. Screen capture of the "prototype windows form" for HyPEP GUI routine development.

- **GUI Development**. The main activity will be developing the object class definitions, which will also be used in numerical coding development. The GUI support routines for component generation and deletion, drag-drop, connection maintenance, flexible layout, etc., will be developed and coded.
- **Component Model Development**. Component specific models will be developed. The models to develop include:
  - VHTR and IHX model
  - Power conversion unit (PCU) T/H model (Brayton cycle and Rankine cycle)
  - HTES T/H model
  - Thermo-chemical model (I-S Cycle). The Node, Link, and Block components will be further developed. The template for the palette, on-screen input/output template for the components will be defined and developed
- **NHDD System Model & Preliminary Calculation**. With the interim version of the HyPEP, a simple NHDD System layout will be modeled and preliminary calculations will be carried out to confirm integrity of the numerical scheme and the ancillary routines.
- **Component Sizing Model Development**. Models will be developed to evaluate the component sizing. Because the model will basically rely on a database, the main task will be to collect and categorize a reliable database.
- **Cost Model Development**. Researchers will develop a simple model (based on database) to calculate the overnight construction cost and an algorithm to calculate simple interest.
- **HyPEP Verification & Validation**. HyPEP will be assessed against established codes such as HYSYS or ASPEN for the program verification and validation.
- **Development of System Optimization Method**. A calculation method/procedure will be developed for the optimization of a nuclear hydrogen production facility. The HyPEP program will be used as the main tool in the method.
- **System Integration**. All the sub-models in the VHTR with PCU and hydrogen plant will be integrated for steady-state analyses. This task includes transient analyses for the control system development.