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Development and Validation of Multidimensional Models of Supercritical CO2 Energy Conversion Systems for Nuclear Power Reactors

Reactor Concepts

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Final Project Report

Development and Validation of Multidimensional Models of Supercritical CO2 Energy Conversion Systems for Nuclear Power Reactors

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Abstract

A general objective of this project was to develop, verify and validate mechanistic multidimensional models of local flow and heat transfer in supercritical carbon dioxide (S-CO2) devices and systems, and to demonstrate the application of the new models to selected components of S-CO2 nuclear energy transport systems. Both steady-state and time-dependent operating conditions have been investigated.
The overall workscope consisted of the following three major parts

- Development, testing and validation of a mechanistic model of forced-convection heat transfer in heated channels cooled using S-CO2 at slightly supercritical pressures.
- Development, testing and verification/validation of a new model of the dynamics of closed-loop S-CO2 heat transport systems.
- Formulation, testing and verification of a mechanistic model for the analysis of flow and pressure distribution in S-CO2 compressors.

The results of the work performed for the project have been documented in several publications.

Statements of Objectives and Accomplishments

<u>Task 1.</u> Development, testing and validation of a mechanistic model of heat transfer in Supercritical CO2 systems

The main objective of this task was to develop, test and validate of a mechanistic model of forced-convection heat transfer in heated channels cooled using S-CO2 at slightly supercritical pressures.

The approach consisted of the following major elements:

- An extensive literature review on the subject of heat transfer for fluids at supercritical pressures.

- Theoretical analysis on the effect of property variations on forced-convection flow and heat transfer in heated channels at slightly supercritical pressures.
- Formulation of a three-dimensional model of variable-property fluid flow and heat transfer in heated channels, and model implementation in the NPHASE-CMFD computer code.
- A detailed analysis of heat transfer in channels using S-CO2 as a working fluid.
- Application of the proposed modeling concept of local heat transfer in supercritical fluids to investigate the effect of variable fluid properties on the operating conditions of different designs of SCWR.

Several challenges have been encountered in conducting the research on this task. One of such challenges dealt with the issue of properly capturing the major mechanisms of combined fluid flow and heat transfer in a manner applicable to a wide range of conditions and with an acceptable level of accuracy. Another example of a challenging issue was concerned with the coupling of CFD RANS-level models with the proposed models of local flow and heat transfer near heated walls.

Practically, all major challenges have been successfully addressed and the associated issues have been resolved. The problems which should be considered as a subject of future work deal with testing and validation of the current model against any new experimental data that may become available, and model application and testing for the geometries of actual heat exchangers used in S-CO2 energy conversion systems.

Detailed results of the work on this task have been documented in the publications:

1. M.Z. Podowski and T. Gallaway, "Hydrodynamic Effects of S-CO2 Property Variations in Nuclear Energy Systems", Proc. Supercritical CO2 Power Cycle Symposium, Boulder, CO, May 24-25, 2011.
2. J. Zhong, S.P. Antal, and M.Z. Podowski, "Thermal Hydraulics Analysis of Heat Transfer in Supercritical Water Reactor Core", Proc. American Nuclear Society 2013 National Student Conference, MIT, Boston, Massachusetts, April 4-6, 2013.
3. J. Zhong, S.P. Antal, and M.Z. Podowski, "Thermal Hydraulics Analysis of Supercritical Water Reactor Core Designs", Paper #583, Proc. 15th Int. Topical Meeting on Nuclear Reactor Thermalhydraulics (NURETH-15), Pisa, Italy, May 12-17, 2013.
4. J. Zhong and M.Z. Podowski, "Toward Mechanistic Modeling of Heat Transfer in Supercritical Fluids", Proc. ANS 2014 Student Conference, Pennsylvania State University State College, Pennsylvania, USA, April 3-5, 2014.
5. M.Z. Podowski, "Recent Advancements in Mechanistic Multidimensional Modeling of Fluid Flow and Heat Transfer in Fluids at Supercritical Pressures", Keynote lecture at Int. Meeting of Specialists on Heat Transfer to Fluids at Supercritical Pressure with Application to Nuclear Reactors and Solar Energy Systems, Manchester, UK, June 30 -July 1, 2014.
6. J. Zhong, S.P. Antal, and M.Z. Podowski, "Impact of Local Property Variations of Reactor Coolant on Cladding Temperature Distribution in Supercritical Water Reactors", *Journal of Power Technologies* (in press), 2014.

7. J. Zhong, S.P. Antal, and M.Z. Podowski. "Mechanistic Modeling of Heat Transfer in Supercritical Carbon Dioxide", ANS Transactions, 2014 ANS Winter Meeting and Nuclear Technology Expo, Washington, DC, Nov. 9-13, 2014 (to be published).
8. J. Zhong and M.Z. Podowski, "New Modeling Concepts of Forced-Convection heat Transfer in Fluids at Slightly Supercritical Pressures", *Nuclear Engineering and Design* (in preparation).

Task 2. Development, testing and validation of a model of the dynamics of S-CO2 heat transport systems.

A general thrust of this task has been on the formulation and analysis of one-dimensional models of closed-loop dynamics for systems using supercritical fluids in general, and supercritical carbon dioxide (S-CO2) in particular.

The major accomplishments are as follows:

- An extensive literature review, focused on the experimental data for S-CO2 flow and heat transfer in closed loop configurations.
- Model derivation for flow transients in such loops, with a specific emphasis on natural-recirculation conditions and parallel-channel heaters.
- The modeling of heat flux distribution along the chiller (heat-rejection heat exchanger).
- The formulation of boundary conditions to account for loop pressure control.
- The formulation of discretized models of the heater, the chiller and the closed loop configuration, for both time- and frequency-domain analyses.
- The formulation of a distributed-parameter model for frequency-domain analysis of natural-circulation closed-loop systems.
- The formulation of a distributed-parameter model for the analysis of "channel-to-channel' instability mode in multiple-parallel-channel systems
- Parametric model testing.
- Selection of experimental data for model validation.
- Comparative calculations of model's predictions against the chosen experimental data sets.
- Qualitative analysis of the proposed mathematical models to formulate generalized stability criteria for closed-loop supercritical-pressure systems.

As in Task-1, several challenges have been encountered again, including those related to model formulation, as well as to testing the effect of variable fluid properties on the response of closed-loop systems. All major issues have been resolved, although the final touch will still require some extra work before the overall results are ready for publication in archival journals.

Detailed results of the work on this task have been, or are going to be, documented in the following publications:

9. W. Smith and M.Z. Podowski, “Theoretical and Computational Analysis of Flow Oscillations in S-CO2 Natural Circulation Loop”, Proceedings of ICAPP’12, Paper 12273, June, 2012, pp.1982-1987.
10. W.C. Smith and M.Z. Podowski, "Modeling and Analysis of Flow-induced Instabilities in Natural-Circulation Closed Loop Super-Critical Fluid Systems", Proc. 15th Int. Topical Meeting on Nuclear Reactor Thermalhydraulics (NURETH-15), Paper#585, Pisa, Italy, May 12-17, 2013.
11. W. Smith and M.Z. Podowski, “Formulation, Testing and Validation of Frequency-Domain and Time-Domain Models of Closed Loop Dynamics for Super-Critical Fluid Systems”, *Nuclear Technology*, in preparation.
12. W. Smith and M.Z. Podowski, “Stability Maps for Parallel-Channel Closed-Loop Systems using Fluids at Supercritical Pressures”, in preparation for submission to *Nuclear Engineering and Design*, 2014

Task 3. Mechanistic modeling and analysis of flow and pressure distribution in Supercritical CO2 systems

The major objectives of this task were to: formulate a complete new DNS-level model of S-CO2 applicable to a wide range of pressures, implement the new model in the PHASTA code, and apply this model in the analysis of a compressor of the type used in the SANDIA loop experiments. The approach used to accomplish these objectives consisted of several steps, as listed below.

- The formulation of a complete detailed thermodynamic model of physical properties of S-CO2, applicable to pressures from slightly supercritical to nearly 20 MPa.
- The development of a numerical algorithm for implementation of this model, including both the propertied themselves and their derivative with respect to both pressure and temperature, in the form of general user routines.
- The formulation of a complete three-dimensional fully-compressible time-dependent model of S-CO2, which uses the thermodynamic properties model mentioned above.
- The implementation of the new model in the PHASTA code.
- Parametric testing of the PHASTA-based model for various geometries and flow conditions.
- The development of an analytical one-dimensional model of S-CO2 flow along variable-area conduits.
- The verification of physical consistency and numerical accuracy of the three dimensional model against the rigorous solutions of the one-dimensional model.
- A comparative analysis between the model of actual properties of S-CO2 and a comparable model of ideal gas (both fully-compressible).
- A comparative analysis between the compressible and incompressible models of S-CO2 for geometries representing simplified versions of the SANDAI compressor.

- The formulation of a detailed three-dimensional CAD model of a compressor, based on the published data for the compressor used in the SANDIA loop.
- A comparative analysis of the complete three-dimensional models of both incompressible and compressible flows along rotating blades of the actual SCO2 compressor.

All major goals of the work for this task have been accomplished. It has been shown that the model of the actual S-CO2 properties, implemented in PHASTA, is both physically correct and numerically accurate. Also, it has been demonstrated that the compressible flow model of S-CO2 implemented in the PHASTA code is consistent and properly predicts the pressure and flow fields in curved channel geometries.

A comparative analysis between three different models of physical properties of CO2 at supercritical pressures for the conditions similar to those encountered in typical compressors has shown that: (a) as long as the conduit geometry results in relatively small velocity changes along the flow, the predictions using an incompressible model (but with all properties other than density corresponding the actual CO2) are very similar to those using a fully compressible model, and (b) the predictions using an equivalent fully compressible model of ideal gas (a very popular approach used in compressor design) are significantly different from those using the actual propertied of S-CO2.

It has been found that the inclusion of blade rotation in complete compressible compressor models introduced profound computational difficulties, including instabilities caused by the effect of both inlet conditions (a transition from stationary to rotating flows) and exit (pressure- and temperature-induced local instabilities in the velocity field). On the other hand, the incompressible model is very stable, while its predictions are not much different from those of the compressible flow model.

Detailed results of the work on this task have been documented in the publications:

13. F. Behafarid and M.Z. Podowski, "Multidimensional Modeling and Simulation of Supercritical CO2 Compressor", ANS Transactions, 2013 ANS Winter Meeting and Nuclear Technology Expo, Washington, DC, Nov. 10-14, 2013.
14. F. Behafarid and M.Z. Podowski, "A Study on Numerical Modeling of Supercritical CO2 Flow in Centrifugal Compressors", Proc. ANS International Embedded Topical Meeting on Advances in Thermal Hydraulics, Reno, NV, June 15-19, 2014.
15. F. Behafarid and M.Z. Podowski, “Modeling and Analysis of Thermo-Fluid Phenomena in Supercritical CO2 Compressors”, to be submitted to *Nuclear Engineering and Design*, 2014.
16. F. Behafarid, M.Z. Podowski and K.E. Jansen, “Numerical Simulation of Supercritical CO2 using Finite Element Method under Extreme Accelerations”, to be submitted to *Physics of Fluids*, 2014.
17. F. Behafarid and M.Z. Podowski, “Formulation and testing of DNS Model of Supercritical CO2 Compressor”, to be submitted to *Journal of Engineering for Gas Turbines and Power,* 2014.