Gas Molecular Diffusion Model Implemented in RELAP5-3D

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Diffusion of gases, important for modeling air ingress into a VHTR is implemented in RELAP5-3D.

Background

A molecular diffusion model was previously added to the code, but was not available in the current version of the code because it was not converted to Fortran 90. The molecular diffusion model was originally implemented in the code to calculate the ingress of air into a VHTR (Very-High Temperature Reactor) following an accident such as a complete depressurization. This ingress of air can result in an oxidation of graphite in the core causing an increased peak clad temperature.

Discussion

To reincorporate the molecular diffusion model into the most recent version of the code, the subroutines that implement the model were first converted to Fortran 90. This involved both the coding and the data. The following subroutines now implement the model:

- DIFGAS
- RDFGAS
- TRAN

Subroutine RDFGAS reads and stores the information. Subroutine TRAN calls DIFGAS immediately after the call to HTADV. Subroutine DIFGAS then calculates the molecular diffusion of gases through the network of RELAP5-3D control volumes.

Searches are made for each control volume to determine into which other control volumes a gas may diffuse. Gas diffusivity is calculated using equations from two sources[1,2]. Effective binary diffusion coefficients between each species of gas and the gas mixture are calculated with Eq. 11-4.1 from Reid[1]. The effective binary coefficient between two species of gas is calculated with Eq. 18.4-25, pp. 571 from Bird[2].

The algorithm assumes that the working fluid is either Helium (He), or light water, H_2O.

Calculations that were used to validate the model previously were performed. The results of the calculation compared favorably with previously obtained results (before the conversion). This model will be available in the next IRUG version release.

Bibliography

1. R. C. Reid, J. M. Prausnitz, T. K. Sherwood , The Properties of Gases and Liquid, 3rd Edition, McGraw-Hill Book Co., 1977.

2. R. B. Byrd, W. E. Stewart, E. N. Lightfoot, Transport Phenomena, ISBN 0 471 07392 X, John Wiley and Sons, New York, NY, USA, 1960.