2-DIMENSIONAL MODELING OF THE COMETARY PHASE TRANSITION WITHIN A RANGE OF TEMPERATURES; N. S. Duxbury, R. H. Brown, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109

The amorphous to crystalline ice phase change (1,2) is crucial for the long-term cometary evolution. The 2-D mathematical model of this phase transition within a range of temperatures is developed. As was shown by physical experiments (3), the phase transition normally occurs over a wide range of temperatures; however, it is customary to refer to a fixed phase transition temperature.

Previous 1-D numerical modeling (4,5,6) considers that all of the latent heat is released at once when the temperature reaches the crystallization value. The model presented considers the non-linear parabolic equation with the liberation of latent heat when the temperature belongs to a chosen interval. The application of the new mathematical approach allows one to omit the presumption of the nearly instantaneous (0.3 sec) phase transition under the fixed temperature (6). It was shown later by laboratory experiments (3) that the crystallization time for the same (136.8°K) phase temperature is nearly 2.9 hours. This time was indicated also in analytical formulae (7).

In the model presented, the speed of the phase transition is defined by the speed of the front (\( \frac{\partial \phi}{\partial t} \)) which is determined from the equation

\[
-Q \frac{\partial \phi}{\partial t} = (k_1 \nabla u_1 - k_2 \nabla u_2, \nabla \phi),
\]

where \( Q \) is the latent heat and \( Q > 0 \).

The condition (1) is non-linear and represents the energy conservation law on the front. The efficient heat capacity for the phase change temperature interval \((u^*-\epsilon, u^*+\epsilon)\) was chosen as

\[
\tilde{c} = \frac{-Q}{2\epsilon} + \left( \frac{c_1 + c_2}{2} \right),
\]

where \( \epsilon \) is the parameter of smoothing. Therefore the enthalpy change satisfies the energy conservation law

\[
\int_{u^*-\epsilon}^{u^*+\epsilon} \tilde{c}(u)du = -Q + \int_{u^*-\epsilon}^{u^*+\epsilon} c(u)du.
\]

This phase transition occurs with the liberation of latent heat \((-Q\) in eq. (1)) while ice transforms to the state with higher temperature. That is why the process is described by the ill-posed inverse parabolic equation in the phase transition interval and parabolic equation beyond this interval. So the problem has to be regularized. A fully implicit scheme was chosen for the direct parabolic equation. The scheme with "weights" \((u^* = \sigma \tilde{u} + (1-\sigma)u, \sigma \ll 0, \sigma - \text{"weight" parameter})\) was applied for the inverse equation.
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The current model also considers inhomogeneous media where phase temperature depends upon $\bar{x}$. This opens perspectives for modelling of the phase transition with the inclusion of the other types of ice into water ice within the cometary core.

References