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Refined Thermal Modelling of a SNF Shipping-Cask Drying Process Analytical and Statistical Approaches

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ABSTRACT

Before being back-filled with an inert gas and as preparation for shipment, a spent-nuclear-fuel shipping cask must usually be vacuum-dried. This process results in an increase in the spent fuel temperature, due to the degradation of heat transport by the cover gas. The drying process is typically modelled by a thermal conduction set to zero in all the shipping-cask free spaces. However, this approach does not take into account heat transfers that occur in a rarefied medium and, therefore, may be extremely conservative.

A first analysis was performed in order to spot the cask areas whose thermal behaviour is modified by the drying process. This analysis involved the calculation of the Knudsen number, defined as the molecular mean-free-path to a representative length scale, for all the free spaces. The only area impacted by the drying process appeared to be the mechanical gap between the fuel basket and the shielding materials. During the drying process, the Knudsen number is actually large enough within the gap to consider the gas as a non-continuous medium. Results and methods coming from the microfluidics area were therefore used to develop a modelling, which is based on a double approach.

First, an analytical approach was used. This approach consists in adding to the Fourier equation a new equation accounting for the thermodynamical non-equilibrium within the gap (Maxwell-Smoluchowski temperature jump). A thermal model, suitable to calculate heat transfers at pressures as low as 1 mbar, was developed.

A second model, based on a statistical approach, was then developed. This model involves the *Direct Simulation Monte Carlo* method, a reference method used for microfluidics calculations. Computer simulations were performed and led to a good agreement with the results obtained by the analytical approach.

INTRODUCTION

Before being back-filled with an inert gas and as preparation for shipment, a spent-nuclear-fuel (SNF) shipping cask must usually be vacuum-dried. This operation is required to prevent aqueous corrosion of the cladding and cask materials. It is also necessary to avoid radiolytic formation of hydrogen.

The vacuum drying process involves lowering the cover gas pressure below the vapor pressure of the water at the drying temperature. The cask is considered to be satisfactorily dry when the system pressure (around 5 mbar) remains constant for a specific time period (usually, around 30 minutes). However, large amounts of residual water may require a fairly long drying time.

This process results in an increase in the spent fuel temperature, due to the degradation of heat transport by the cover gas. In order to assess the consequences of the cladding creep during transportation, a good knowledge of this temperature increase is necessary. The drying process is usually modelled by a thermal conduction set to zero in all the shipping-cask free spaces. However, this approach does not take into account heat transfers that occur in a rarefied medium and, therefore, may be extremely conservative.

The aim of this paper is to present a new method to better assess the cladding temperatures induced by the drying process.

PHYSICAL PHENOMENA OCCURRING IN THE DRYING PROCESS

During the drying process, the inner-cask air at a near-atmospheric pressure is replaced by an air/water-vapor mixture at ~6 mbar. In other words, a radiation-transparent, continuous medium is replaced by a translucent medium, which may not behave as a continuous medium any more.

Therefore, two issues have to be addressed here. The first one concerns the radiative properties of the air/water-vapor mixture at a 6-mbar pressure. This is not a critical issue and it can easily be shown that, for these conditions, the mixture can still be considered as a transparent medium.

The second one concerns the conductive properties of the gas mixture, especially in the smallest cavities of the shipping cask, where the hypothesis of a continuous medium may not be valid any more. This is a real critical issue, and it will be the main focus of this paper.

CONDUCTIVE PROPERTIES OF THE GAP GAS – ANALYTICAL APPROACH

A key parameter in characterizing the degree of rarefaction of the gas and the validity of the continuum hypothesis in the Navier-Stokes equations is the *Knudsen number* (*Kn*). *Kn* is the ratio of the mean free path of the gas molecules, λ, to the characteristic dimension of the flow geometry, L_c:

$$Kn = \frac{\lambda}{L_c} \tag{1}$$

For an ideal gas, λ can be related to the temperature, T, and pressure, p, via the following equation, where k is Boltzmann's constant and d is the diameter of the molecules:

$$\lambda = \frac{kT}{\sqrt{2}\pi p d^2} \tag{2}$$

A classification of the various stages of rarefaction has been proposed by Schaaf and Chambré [1], based upon the magnitude of the local Knudsen number:

$$\begin{cases} Kn \le 10^{-2} & : \text{ continuum flow,} \\ 10^{-2} \le Kn \le 10^{-1} & : \text{ slip flow,} \\ 10^{-1} \le Kn \le 10 & : \text{ transition flow,} \\ Kn > 10 & : \text{ free-molecular flow.} \end{cases}$$

For $Kn \le 10^{-2}$, the continuum hypothesis is appropriate and the flow can be described by the Navier-Stokes equations using conventional no-slip boundary conditions. In other words, in such conditions, for a gas restricted by a solid surface, the surface temperature and the temperature of the gas near the surface are equal.

For $10^{-2} \le Kn \le 10^{-1}$, the Navier-Stokes equations are still considered to offer a reasonable description of the flow, provided a temperature-jump boundary condition is implemented between the gas and the solid. This boundary condition (also referred to as the *Maxwell-Smoluchowski temperature-jump*) accounts for the thermodynamic non-equilibrium near the solid surface, in a zone called the *Knudsen layer*.

For $10^{-1} \le Kn \le 10$, the continuum assumption in the Navier-Stokes equations begins to break down and alternative methods of analysis are required. The gas-kinetic equations derived by Boltzmann provide a good way to describe the flow, although these equations may be extremely complicated to solve. Another convenient way is to use the particle-based *Direct Simulation Monte Carlo* (DSMC) statistical approach, developed by Bird [2].

For $Kn > 10$, the continuum approach breaks down completely. In such conditions, molecules reflected from a solid surface travel many length scales before colliding with other molecules. In this case, the DSMC method still provides a good tool to analyse such flows.

Knudsen numbers of the inner-cask flows

Equation (2) establishes that, during the drying process, λ cannot exceed a value of 5.10^{-5} m. In other words, all the inner-cask spaces will still experience a continuum-flow regime, unless their characteristic dimension is less than 5 millimeters (i.e., $Kn < 0.01$).

The shipping casks come in different designs. However, they typically consist of a basket loaded with SNF, and a neutron and gamma shielding. For operational flexibility, the basket is often removable. Therefore, a mechanical gap takes place between the basket and the shielding inner-shell, whose thickness may be significantly less than 5 millimeters. Because the Knudsen number is in this case greater than 0.01, a slip-flow regime must be considered.

For a mechanical gap thickness less than 0.5 mm (i.e., $Kn > 0.1$), multiple points of contact are here assumed to appear between the basket and the shielding shell, leading to a significant conductive heat transfer. Besides the continuum-flow regime, the slip-flow regime is therefore the only regime that is considered in the present analysis.

Development of a simplified model

For a gas temperature, T_G, and a solid temperature, T_W, the temperature-jump boundary condition reads [3]:

$$T_G - T_W = \zeta_T \frac{\mu}{P}\left(\frac{2kT_W}{m}\right)^{1/2} \cdot \frac{q''}{k_G} \tag{3}$$

where μ is the dynamic viscosity, P the local pressure, k_G the thermal conductivity, and m the molecular mass of the gas; k is Boltzmann's constant, and q'' the heat flux transferred from the basket to the gap.

The dimensionless constant ζ_T is called the *temperature-jump coefficient*, whose value is obtained by solving the Boltzmann equation in the Knudsen layer. Many papers were written on this topic [3] [4], and, because the computation of ζ_T is not the primary focus of this paper, the value used in the calculations is just stated here:

$$\zeta_T = 2.0 \tag{4}$$

A 1-D model of the shipping cask is then developed. It includes the basket, the mechanical gap, and the shielding, as represented in Figure 1.

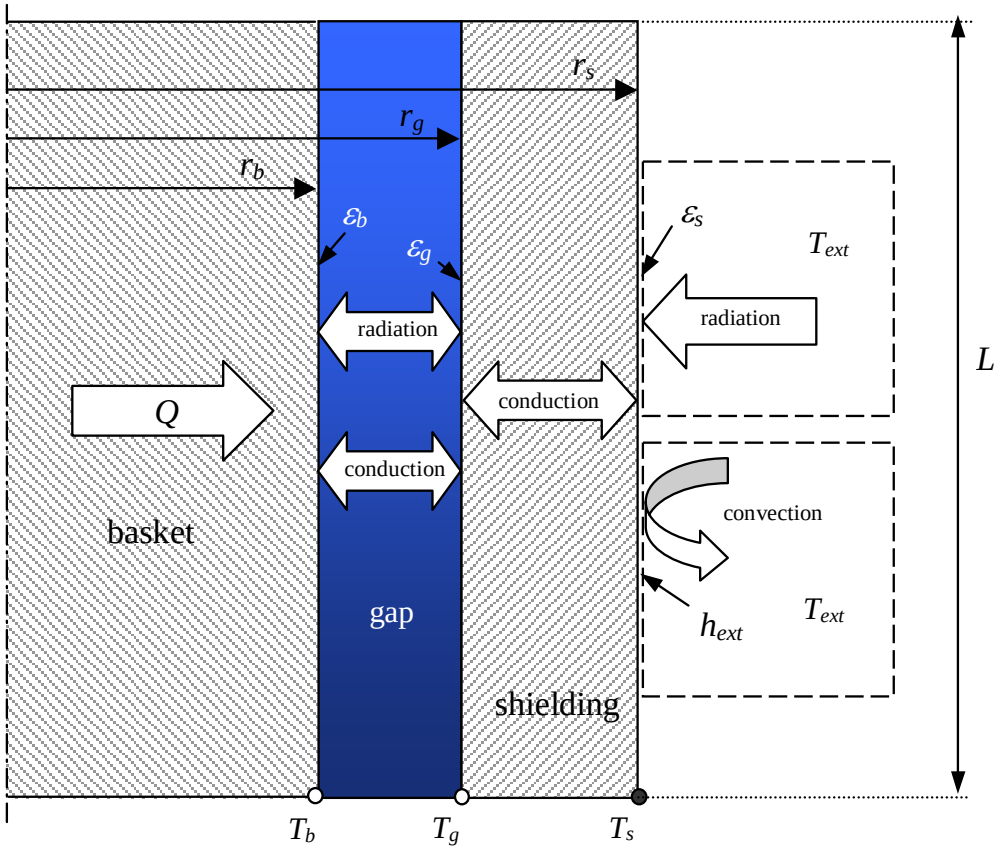

Figure 1. Simplified Thermal Model of the Shipping Cask

This simplified problem has five unknowns: the shielding outer-surface temperature, T_s, the shielding inner-surface temperature, T_{gW}, the gas temperature near the shielding, T_{gG}, the gas temperature near the basket, T_{bG}, and the basket temperature, T_{bW}. The outside air and the surroundings are assumed to be at temperature T_{ext}.

The unknown temperatures can be easily calculated by the following heat balances:

$$\begin{cases} Q = 2\pi k_{mix} L.\dfrac{T_{bG} - T_{gG}}{\ln(\dfrac{r_g}{r_b})} + 2\pi r_b L\sigma.\dfrac{(T_{bW}^4 - T_{gW}^4)}{\dfrac{1}{\varepsilon_b} + \dfrac{r_b}{r_g}(\dfrac{1}{\varepsilon_g} - 1)} & (5) \\ Q = 2\pi k_s L.\dfrac{T_{gW} - T_s}{\ln(\dfrac{r_s}{r_g})} & (6) \\ Q = 2\pi r_s L h_{ext}.(T_s - T_{ext}) + 2\pi r_s L\sigma\varepsilon_s.(T_s^4 - T_{ext}^4) & (7) \\ Q = 2\pi k_{mix} r_b L.\dfrac{T_{bW} - T_{bG}}{\zeta_T \dfrac{\mu_{mix}}{P_{mix}}\left(\dfrac{2kT_{bW}}{m_{mix}}\right)^{1/2}} = 2\pi k_{mix} r_g L.\dfrac{T_{gG} - T_{gW}}{\zeta_T \dfrac{\mu_{mix}}{P_{mix}}\left(\dfrac{2kT_{gW}}{m_{mix}}\right)^{1/2}} & (8) \end{cases}$$

where Q is the total heat flux transferred from the SNF through the basket; k_{mix} is the thermal conductivity of the air/water-vapor mixture and k_s the thermal conductivity of the shielding material; ε_b, ε_g, ε_s are the emissivities of the basket, the shielding inner-surface, and the shielding outer-surface respectively; h_{ext} is the convective heat transfer coefficient between the shielding outer-surface and the exterior air; σ is Stefan's constant.

Results

Table 1 presents the temperature increases induced by the drying process. The methodology described above was applied to the following data, which can be considered as representative of a SNF shipping-cask loaded with twelve SNF, and with a gas assumed to be pure water vapor:

$$\begin{cases} k_s = 39\ \text{W.m}^{-1}.°\text{C}^{-1}, \\ \varepsilon_b = 0.3,\ \varepsilon_g = 0.5,\ \varepsilon_s = 0.8, \\ P_{mix} = 10^2\ \text{Pa},\ h_{ext} = 45\ \text{W.m}^{-2}.°\text{C}^{-1},\ T_{ext} = 30°\text{C}, \\ L = 3.66\ \text{m},\ r_b = 0.608\ \text{m},\ r_g = 0.610\ \text{m},\ r_s = 1.06\ \text{m}. \end{cases}$$

In Table 1, T_{max} is the maximum fuel rod temperature. This temperature was computed by use of a specific SNF model, which was proposed by Manteufel and Todreas [5].

The results show that the drying process induces an increase in the maximum fuel rod temperature of about 20°C for a heat generation rate of 3,000 W per fuel assembly. This increase is about 25°C for a heat generation rate of 5,000 W per fuel assembly.

Table 1. Impact of the Drying Process - Temperature Increases Within the Cask (°C)

Q_{SNF}	3000 W	5000 W
ΔT_{max}	**20.4**	**24.7**
ΔT_{bW}	34.0	40.8
ΔT_{bG}	15.2	6.6
ΔT_{gG}	3.6	6.0
ΔT_{gW}	-6.6	-11.1
ΔT_s	0.0	0.0

CONDUCTIVE PROPERTIES OF THE GAP GAS – STATISTICAL APPROACH

The DSMC method, developed by Bird [2] and mentioned in the previous paragraph, was used by means of a computer code to simulate the heat transfers by conduction within the gap. The method was applied to a gap first filled with pure air, and then filled with an air/water-vapor mixture. A preliminary step consisted for each case in choosing the most appropriate collision model.

Gap filled with pure air

The *Variable Soft Sphere* [5, 6] model was used here for both nitrogen and oxygen. The aim of this model was to reproduce the phenomenological transport coefficients under the hypothesis of inverse-power-law or Lennard-Jones potential in a collision between two molecules. The rotational energy of the molecules and a relaxation by a collision process was considered as well [2]. DSMC simulations of the heat conduction in the continuous regime (i.e., for small *Kn* values) were performed, in order to infer the thermal conductivity of the gap gas. The calculated values were then found consistent with the experimental ones.

Gap filled with an air/water-vapor mixture

The problem is more complex with water, and generally with polar molecules. The simple Lennard-Jones potential, with a repulsive force at small distances and an attractive force at large distances, is indeed not appropriate to deal with such molecules. A Stockmayer potential including a polarization term due to an electrostatic contribution is then necessary. This was done by considering a *Generalized Soft-Sphere* model [8], which was implemented in the DSMC code. With this model, water vapour and air/water-vapor mixtures could be analysed as well. As above, calculated values of thermal conductivities in the continuous regime were found consistent with experimental ones.

Strategy for the simulation

The parameters of the problem, for a given gas mixture, are the shielding inner-surface temperature, T_{gW}, the basket temperature, T_{bW}, the gap size $\delta = r_g - r_b$ (where r_b is assumed fixed), and the gas pressure P within the gap.

The different relations that were used here are the following ones:

$$\begin{cases} Kn = \dfrac{\lambda_{mix}}{\delta} & (9) \\ n\lambda_{mix} = \displaystyle\sum_{p=1}^{s} \frac{x_p}{\displaystyle\sum_{q=1}^{s} x_q \sigma_{pq} \left(1 + \frac{m_p}{m_q}\right)^{1/2}} & (10) \\ n = P/kT & (11) \\ T = (T_{gW} + T_{bW})/2 & (12) \end{cases}$$

where λ_{mix} is the mean free path of the gas mixture including s species [2], x_i and m_i are the molar fraction and mass of species i respectively, and σ_{ij} is the total cross section between species i and j. The total density is estimated using the mean value of the wall temperatures. P varies from 1 to 6 mbar and δ from 0.015 mm to 2 mm. The wall temperatures vary from 340 K to 700 K.

The strategy chosen here was to find the most simple way to present the results, knowing that several parameters vary, as mentioned above.

Let Q_D be the conductive heat flux issued from the DSMC simulations and Q_C the conductive heat flux that would be observed for a continuous regime.

Q_C can here be expressed as:

$$Q_C = 2\pi L k_{mix}(T)\frac{T_{bW} - T_{gW}}{\ln(\frac{r_g}{r_b})} \tag{13}$$

where k_{mix} is the thermal conductivity of the gas mixture, computed at the mean temperature, T, defined by Equation (12).

It was established that, for a given gas mixture, the ratio Q_D/Q_C could be represented in terms of the Knudsen number, *independently* of the temperatures, as shown in Figure 2. It could also be proven that, in the range of temperatures considered, the limit of Q_D/Q_C is zero, when *Kn* tends towards infinity. It is exactly what is shown in Figure 2.

After fitting theses curves, the system of Equations (5) through (8) was replaced by a new system, where the first term of Equation (5) is replaced by Q_D and Equation (8) is cancelled. Then, the new system was solved and led to the results presented in Table 2. In order to compare the results, the temperature increases obtained with the analytical approach were also recalled therein.

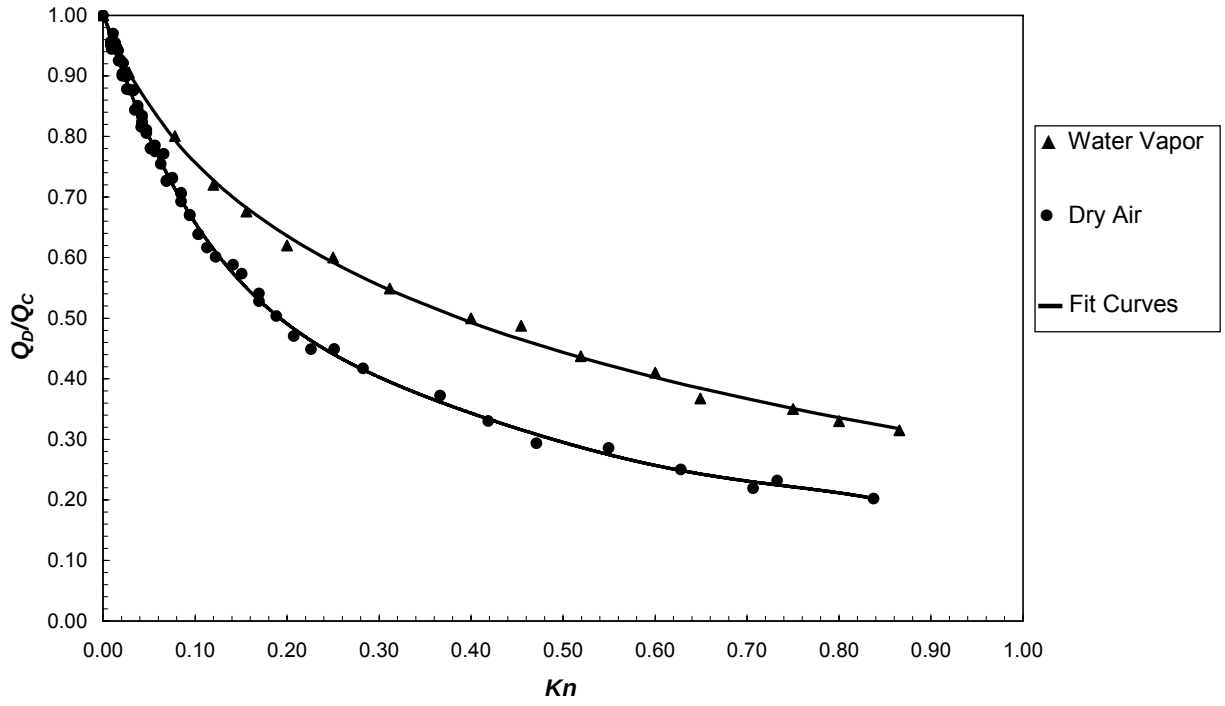

Figure 2. Reduced Heat Flux Q_D/Q_C vs. the Knudsen Number for Dry Air and Water Vapor

Table 2. Impact of the Drying Process - Temperature Increases Within the Cask (°C)

	Drying Process – Analytical Approach		Drying Process – Statistical Approach	
Q_{SNF}	3000 W	5000 W	3000 W	5000 W
ΔT_{max}	**20.4**	**24.7**	**24.7**	**27.0**
ΔT_{bW}	34.0	40.8	40.9	44.4
ΔT_{gW}	-6.6	-11.1	-0.1	-0.2
ΔT_{s}	0.0	0.0	-0.2	-0.1

CONCLUSIONS

A new method to better assess the cladding temperatures induced by the drying process within a SNF shipping-cask was presented in this paper. Two kinds of models, including analytical and statistical approaches, were developed and led to consistent results. This consistency may be considered as a validation of the analytical approach, which is convenient to use in engineering calculations.

However, this is just a first step towards a comprehensive modelling of the drying process. A 3-D model, which involves teams both at CEA and EDF in France, is indeed being developed. This model will simulate the dilatation of the materials and the progressive closing of the mechanical gap. Within the gap, a more complex model of heat transfers within a rarefied medium will be implemented. This model, based on DSMC calculations, will be able to deal with different kinds of flow regimes, associated with a wide range of Knudsen numbers.

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REFERENCES

[1] Schaaf SA, Chambré PL. *Flow of Rarefied Gases*. Princeton University Press: Princeton, 1961.
[2] Bird GA. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford Science Publications, Clarendon Press: Oxford, 1994.
[3] Sharipov F, Kalempa D. Velocity Slip and Temperature Jump Coefficients for Gaseous Mixtures. Temperature Jump Coefficient. *International Journal of Heat and Mass Transfer* 2005; **48**:1076–1083.
[4] Sharipov F. Application of the Cercignani–Lampis Scattering Kernel to Calculations of Rarefied Gas Flows. Slip and Jump Coefficients. *European Journal of Mechanics - B/Fluids* 2003; **22**:133–143.
[5] Manteufel RD, Todreas NE. Effective Thermal Conductivity and Edge Conductance Model for a Spent-Fuel Assembly. *Nuclear Technology* 1994; **105**:421–440.
[6] Koura K., Matsumoto J. Variable Soft Sphere Molecular Model for Inverse-Power-Law or Lennard-Jones Potential. *Phys. Fluids* 1991; A **3**:2459–2465.
[7] Koura K., Matsumoto J. Variable Soft Sphere Molecular Model for Air Species. *Phys. Fluids A* 1992; **4**:1083–1085.
[8] Fan Jing. A Generalized Soft-Sphere Model for Monte Carlo Simulation. *Phys. Fluids* 2002; **14**:4399–4405.