International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

IMPROVED THERMAL MODELLING OF A SNF SHIPPING-CASK DRYING

Didier Colmont
EDF R&D
6 quai Watier
78401 Chatou Cedex, France
didier.colmont@edf.fr

Philippe Roblin, Caroline Guérin
CEA
DEN/DM2S
Centre d'Etudes de Saclay
91191 Gif-sur-Yvette Cedex, France
philippe.roblin@cea.fr, caroline.guerin@cea.fr

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 aim of this paper is to present a method to assess this temperature increase.
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.
Using the results of both approaches, an effective thermal conductivity of the gap gas could be inferred and used in a 3-D thermomechanical model of the shipping cask.

Key Words: Shipping-Cask, Modelling, Drying, Microfluidics.

1. 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 6 mbar) remains constant for a specific time period (usually, around 30 minutes). However, large amounts of residual water may require a much longer 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.

This paper presents a new method to better assess the cladding temperatures induced by the drying process.

2. 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 is the main focus of this paper.

3. 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, by means of 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:

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

For $Kn \leq 10^{-2}$, 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 $10^{-2} \leq Kn \leq 10^{-1}$, 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 $10^{-1} \leq Kn \leq 10$, 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.

3.1. 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 for a gas pressure of 5 mbar. 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 and making it unnecessary to deal with the transition-flow regime.

Besides the continuum-flow regime, the slip-flow regime is therefore the only regime that is considered in the present analysis.

3.2. Development of a Simplified Steady-State 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, reporting values of ζ_T close to each other [3, 4], and, because the computation of this coefficient 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.

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}),
- the basket temperature (T_{bW}).

The outside air and the surroundings are assumed to be at temperature T_{ext}.

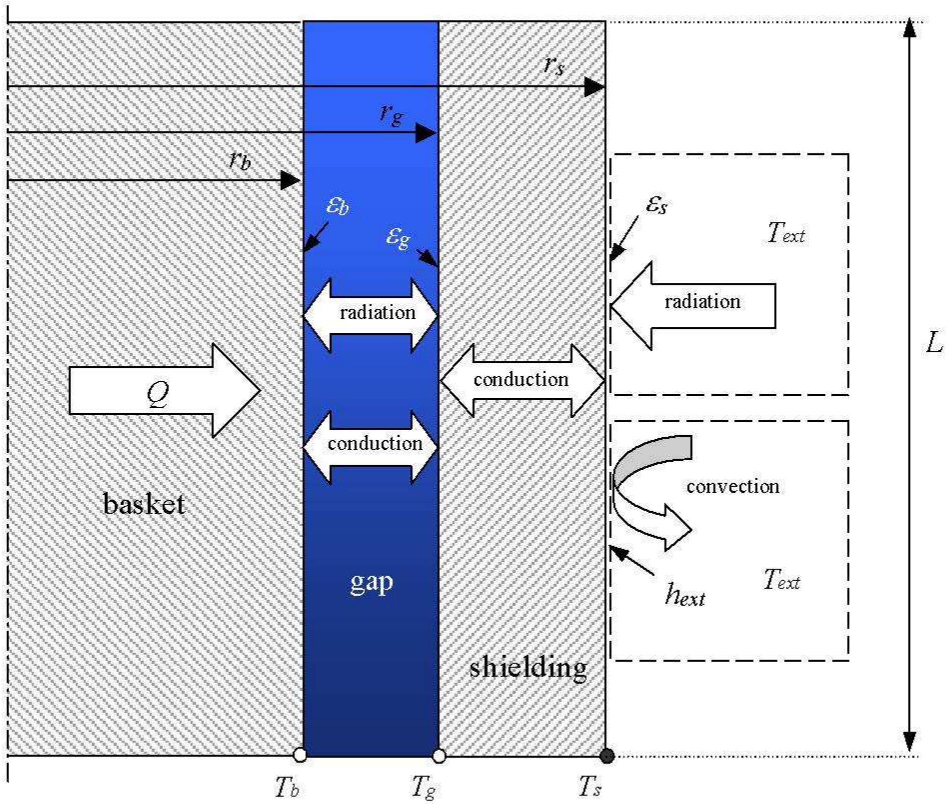

Figure 1. Simplified Thermal Model of the Shipping Cask

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

$$Q = 2\pi k_{mix} L.\frac{T_{bG} - T_{gG}}{\ln(\frac{r_g}{r_b})} + 2\pi r_b L\sigma.\frac{(T_{bW}^4 - T_{gW}^4)}{\frac{1}{\varepsilon_b} + \frac{r_b}{r_g}(\frac{1}{\varepsilon_g} - 1)} \quad (5)$$

$$Q = 2\pi k_s L.\frac{T_{gW} - T_s}{\ln(\frac{r_s}{r_g})} \quad (6)$$

$$Q = 2\pi r_s L h_{ext}.(T_s - T_{ext}) + 2\pi r_s L\sigma\varepsilon_s.(T_s^4 - T_{ext}^4) \quad (7)$$

$$Q = 2\pi k_{mix} r_b L.\frac{T_{bW} - T_{bG}}{\zeta_T \frac{\mu_{mix}}{P_{mix}}\left(\frac{2kT_{bW}}{m_{mix}}\right)^{1/2}} = 2\pi k_{mix} r_g L.\frac{T_{gG} - T_{gW}}{\zeta_T \frac{\mu_{mix}}{P_{mix}}\left(\frac{2kT_{gW}}{m_{mix}}\right)^{1/2}} \quad (8)$$

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.

3.3. Results

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 assemblies:

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

In addition to these data, the pressure of the air/water-vapor mixture, P_{mix}, was taken equal to 1 mbar. It should be noted, however, that so low a value for P_{mix} is not recommended for the drying process. The French nuclear safety authority requires indeed that this pressure be above 6 mbar to prevent any formation of ice. Lower values have nevertheless been experienced in the past and may still be experienced in incidental conditions, and this is why a value of 1 mbar was considered in the present paper.

Table I presents the calculated increase in temperature at various locations within the cask resulting from the drying process, where ΔT_{max} is the calculated increase in the fuel rod temperature. T_{max} 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. Note that, for both cases, the shielding inner-surface temperature, T_{gW}, is lowered during the process, since the temperature-jump boundary condition is equivalent to a thermal resistance that isolates the shielding from the hottest parts of the cask.

Table I. 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

4. CONDUCTIVE PROPERTIES OF THE GAP GAS – STATISTICAL APPROACH

4.1. Method

The DSMC method, developed by Bird [2] as previously discussed, was used by means of a computer code to simulate the heat transfers by conduction in steady state within the gap.

This method accounts for the gas dynamics by solving the Boltzmann equation. It consists in tracking simultaneously millions of particles, and calculating collisions using a probabilistic technique. This method can be applied to problems with complex molecular models, including internal energy relaxations or chemical reactions. Because of the prohibitive computational time required when dealing with large gas densities, the DSMC method is generally used for rarefied gas. Nevertheless, the recent implementation of the method by the French Atomic Energy Commission (CEA) on massively parallel machines allows to deal with continuum flows.

In the simulations, the molecules were submitted to diffuse reflections at the gap walls. They were then reemitted with a Maxwellian function calculated at the wall temperature. The balance between the fluxes of incident and reflected total energies due to particle impacts finally provided the wall heat fluxes.

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 molecule collision-model. This step is presented in more details in the next paragraphs.

4.1.1. Gap filled with pure air

The *Variable Soft Sphere* [6, 7] 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.

4.1.2. 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.

4.2. 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:

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

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.

4.3. Results

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:

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

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

For a given gas mixture, representing the ratio Q_D/Q_C in terms of Kn is a convenient way to show the degradation of heat transfers for large Knudsen numbers, as shown in Figure 2. It could 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 these 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 II. In order to compare the results, the temperature increases obtained with the analytical approach were also recalled therein.

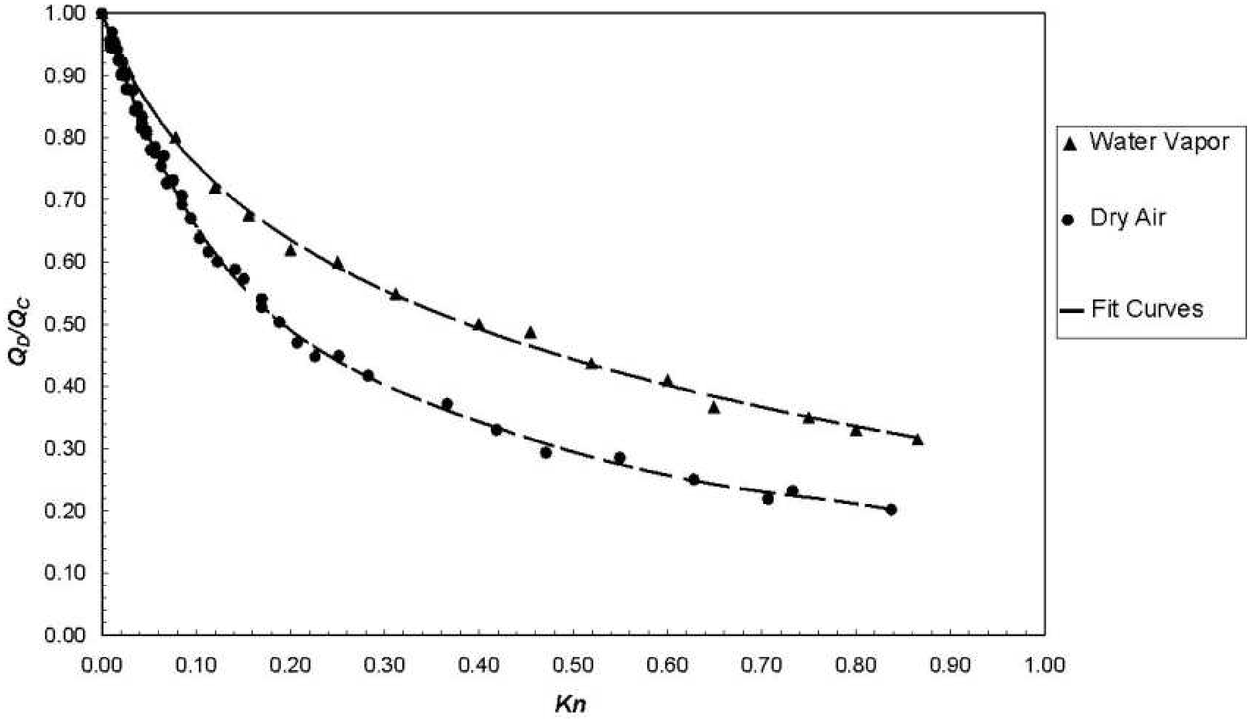

Figure 2. Reduced Heat Flux Q_D/Q_C vs. Knudsen Number

A good agreement between the two approaches was noted for ΔT_{max}, which is the relevant quantity for analysing cladding creep. This agreement may therefore be considered as a validation of both approaches to calculate the thermal impact of the drying process on the fuel claddings.

Table II. 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

5. 3-D THERMOMECHANICAL CALCULATIONS OF THE SHIPPING CASK

With the validation of the approaches described here above, the thermal analysis of the shipping-cask drying process can be put a step further. Under a heat flux, a shipping cask is indeed not a static system. The thermal expansion of the materials will lead to a progressive closing of the mechanical gap, raising the Knudsen number, while creating thermal bridges between the basket and the shielding.

5.1. Thermomechanical Model

Several 3-D thermomechanical transient calculations of the shipping cask were performed using *CAST3M*, a finite-element code developed by the CEA [9]. The local values of the gap thickness were calculated from the mechanical strains due to the thermal expansion of the basket and the shielding by means of an iterative process, since the temperature field strongly depends on this thickness. Unilateral contacts were imposed between the basket and the shielding, in order to avoid their interpenetration. The minimum gap thickness was taken equal to the expected roughness of the surfaces.

In the calculations, the gap gas was represented by an effective thermal conductivity, which was inferred from the results presented in Figure 2. For a given gap thickness, the fit curves presented in Figure 2 provide indeed the correction to apply to the gas thermal conductivity at atmospheric pressure to account for rarefaction effects.

5.2. Results

Table III presents the calculated increase in the maximum fuel rod temperature, ΔT_{max}, obtained from the thermomechanical analysis. ΔT_{max} was calculated here for heat generation rates of 3,000 W and of 5,000 W per fuel assembly and for a gap filled either with water vapor or with pure air.

The results show that ΔT_{max} is less than one half of what was predicted by steady-state calculations, leading to better margins for any assessment of the cladding creep during transportation.

Table III. Thermomechanical Calculations - Temperature Increases Within the Cask (°C)

Q_{SNF}	3000 W	5000 W
ΔT_{max} (Water Vapor)	8	9
ΔT_{max} (Air)	8	5

6. 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 steady-state models, including analytical and statistical approaches, were developed and led to consistent results. This consistency was considered as a validation of the analytical approach, which is convenient to use in engineering calculations.

A 3-D thermomechanical model was developed, putting the analysis a step further. This model simulated the progressive closing of the mechanical gap and evaluated the heat transfer within the gap, based on a variable Knudsen number. The temperature increases calculated with this model were much more realistic and smaller than the ones predicted by the steady-state calculations.

ACKNOWLEDGMENTS

The authors would like to acknowledge Jacques Segré and Henri Paillère (CEA/DEN Saclay) for their support.

REFERENCES

1. S. A. Schaaf, P. L. Chambré, *Flow of Rarefied Gases,* Princeton University Press, Princeton, USA (1961).
2. G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, Oxford, UK (1994).
3. F. Sharipov, D. Kalempa, “Velocity Slip and Temperature Jump Coefficients for Gaseous Mixtures. Temperature Jump Coefficient,” *International Journal of Heat and Mass Transfer*, **48**, pp.1076–1083 (2005).
4. F. Sharipov, “Application of the Cercignani–Lampis Scattering Kernel to Calculations of Rarefied Gas Flows. Slip and Jump Coefficients,” *European Journal of Mechanics - B/Fluids*, **22**, pp.133–143 (2003).
5. R. D. Manteufel, N. E. Todreas, “Effective Thermal Conductivity and Edge Conductance Model for a Spent-Fuel Assembly,” *Nuclear Technology*, **105**, pp.421–440 (1994).
6. K. Koura, J. Matsumoto, “Variable Soft Sphere Molecular Model for Inverse-Power-Law or Lennard-Jones Potential,” *Phys. Fluids A*, **3**, pp.2459–2465 (1991).
7. K. Koura, J. Matsumoto, “Variable Soft Sphere Molecular Model for Air Species,” *Phys. Fluids A*, **4**, pp.1083–1085 (1992).
8. J. Fan, “A Generalized Soft-Sphere Model for Monte Carlo Simulation,” *Phys. Fluids,* **14**, pp.4399–4405 (2002).
9. P. Verpeaux, A. Millard, T. Charras, *CASTEM 2000, une approche moderne du calcul des structures*, Calcul des structures et intelligence artificielle, Editions Pluralis, Paris, France (1989).