

Research Article

Study on the Impact of Thermal Agitation on Doppler Coefficient in Epithermal Range for Gd-Bearing Fuel

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The impact of thermal agitation on Doppler coefficient for Gd-bearing fuel was analyzed. It was found through the analysis that the impact increases when a small amount of Gd_2O_3 is added to pure UO_2 fuel although the impact decreases for a large amount of Gd_2O_3 . This tendency was discussed with the usage of simplified expression for the difference of Doppler coefficient. The simplified expression was used to consider the tendency, and it was revealed that the tendency mainly comes from the rapid decrement of multiplication factor and the relatively slow decrement of the magnitude of sensitivity coefficient of U-238 capture cross section at low Gd_2O_3 concentration. Similar tendency which shows a maximum impact on Doppler coefficient at interior concentration is expected for other UO_2 fuel with a slight content of strong absorber. This indicates that Doppler coefficient of UO_2 fuel system with low content of strong absorber should be analyzed carefully by considering thermal agitation in epithermal range.

1. Introduction

Scattering kernel used in epithermal range is usually treated as the asymptotic model in solving the slowing down equation, which does not take thermal agitation into account. If the targets are scatterings of light isotopes, the asymptotic model is appropriate since the change of scattering kernel by thermal agitation is trivial. But for heavy isotopes, the asymptotic model is not appropriate for scattering kernel especially in epithermal range [1] where Doppler effect is remarkable in thermal reactor. Therefore, the impact of thermal agitation on Doppler coefficient has been investigated by many researchers [2–5]. And a simplified treatment of the exact scattering model for deterministic slowing down equation was also developed to reduce the huge computational cost. This simplified treatment called Upscattering Approximation (UA) method [6] was applied to GROUPE module of the NJOY [7] system and was verified through the comparison of

impact on Doppler coefficient with other reported calculation results [6].

Many evaluations were performed by many researchers but the target composition to evaluate Doppler coefficient is mainly UO_2 without any poison. As easily expected, the addition of poison such as Gd_2O_3 to UO_2 fuel causes the change in multiplication factor and also causes the change in Doppler coefficient by the increment of capture rate of the poison. Thus, it is expected that the impact of thermal agitation on Doppler coefficient varies as a function of poison content in UO_2 fuel.

The purpose of this paper is to evaluate the impact of thermal agitation on the Doppler coefficient for Gd-bearing fuel and to reveal the mechanism of the impact of thermal agitation on Doppler coefficient in Gd-bearing fuel. Section 2 deals with the evaluation of the impact for Gd-bearing fuel for various Gd_2O_3 concentrations. Section 3 shows detailed calculation results to describe the dependence of the impact

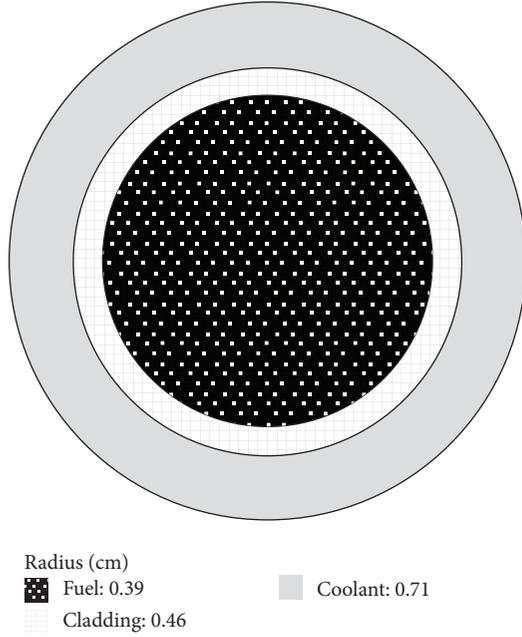


FIGURE 1: Pin cell model.

on Gd_2O_3 concentration. Discussions and conclusions are summarized in Sections 4 and 5, respectively.

2. Calculation of Impact of Thermal Agitation on Doppler Coefficient

The calculation procedure and the calculation results are described in this chapter.

2.1. Calculation Procedure. The calculation geometry is modeled from conventional PWR cell for 4.8 wt% enriched UO_2 fuel with Gd_2O_3 as shown in Figure 1 and Table 1. Fuel temperature is changed from 600 to 900 K and cladding and coolant temperature are unchanged to evaluate Doppler coefficient.

The Doppler reactivity is calculated from two multiplication factors of different fuel temperatures as

$$D.C_{\text{method}} = \frac{(1/k_{\text{low,method}} - 1/k_{\text{high,method}})}{\Delta T}, \quad (1)$$

method = asymptotic model, exact model,

where k_{low} and k_{high} are multiplication factors calculated at low temperature and high temperature, respectively, and ΔT shows the difference between low and high temperatures. The impact of Doppler coefficient is obtained as the relative difference of Doppler coefficient between asymptotic model and exact scattering model.

2.2. Calculation Results. The calculation is performed by continuous energy Monte Carlo code MVP which can handle thermal agitation in epithermal range [8] with JENDL-4.0

TABLE 1: Calculation conditions.

Fuel	
Material	UO_2 with Gd_2O_3
U-235 enrichment	4.8 wt%
Gd_2O_3 concentration	0~20 wt% using following Gd vector
	Gd-152: 0.2 wt%
	Gd-154: 2.2 wt%
	Gd-155: 14.8 wt%
	Gd-156: 20.5 wt%
	Gd-157: 15.6 wt%
	Gd-158: 24.8 wt%
	Gd-160: 21.9 wt%
Temperature	600 K, 900 K
Cladding	
Material	Zircalloy-4
Temperature	600 K
Coolant	
Material	H_2O
Temperature	600 K
Boundary condition	White reflection

TABLE 2: Impact evaluated by MVP for various Gd_2O_3 concentrations.

Gd_2O_3 concentration [wt%]	Impact on Doppler coefficient [%]	Error [%1 σ]
0	8.1	\pm 0.3
0.2	10.6	\pm 0.5
2	9.9	\pm 0.7
5	8.9	\pm 0.7
10	7.7	\pm 0.7
20	5.6	\pm 0.7

library [9]. The impact calculated by 10^9 histories is summarized in Table 2. Table 2 shows that the impact increases by adding small amount of Gd_2O_3 to pure UO_2 fuel and the impact decreases by adding large amount of Gd_2O_3 (10~20 wt%). The smaller impact at high Gd_2O_3 concentration can be explained by smaller amount of U-238 which is the main isotope to cause Doppler reactivity. On the other hand, the impact at low Gd_2O_3 concentration may be enhanced compared to that at pure UO_2 case. Further evaluation is necessary to reveal the mechanism of the enhanced impact at low Gd_2O_3 concentration, but detailed evaluation was performed by deterministic method to reveal the mechanism because the statistical error by stochastic method will bring the ambiguity to consider the mechanism.

3. Detailed Evaluation of Impact

The calculation process and the calculation results for detailed evaluation of the impact are described in this chapter.

TABLE 3: Impact evaluated by UA method for various Gd_2O_3 concentrations.

Gd_2O_3 concentration [wt%]	Impact on Doppler coefficient [%]
0	9.4
0.2	12.2
2	12.0
5	10.6
10	8.5
20	5.6

3.1. Calculation Process. Calculation geometry and calculation conditions are the same as previous chapter. Deterministic evaluations of Doppler coefficient with considering thermal agitation were performed by the following process. The multiplication factor with considering thermal agitation is evaluated with the usage of sensitivity coefficients for the multiplication factor and the relative difference of cross sections between asymptotic model and exact model as expressed in

$$k_{UA} = k_{conv} \cdot \left(1 + \sum_g d^g \cdot S^g \right), \quad (2)$$

where k_{conv} is a multiplication factor calculated by SRAC2006 [10] based on asymptotic model and g is the suffix of energy group and S^g is the sensitivity coefficient for multiplication factor calculated by SRAC2006 and SAINT-II [11] system and d^g is calculated as the relative difference of cross section between asymptotic model and UA method evaluated by NJOY with ENDF-B/VII.0 [12]. Here the exact model is replaced as UA method which has developed and verified to evaluate the cross section with considering thermal agitation for various fuel compositions [6]. The sensitivity coefficient S^g is defined as the ratio of relative change of multiplication factor to the relative change of cross section. Thereby the sensitivity coefficient is expressed as

$$S^g = \frac{dk/k}{d\sigma^g/\sigma^g}, \quad (3)$$

where σ^g is group-averaged cross section of energy group g . The impact of thermal agitation on Doppler coefficient was evaluated by using the multiplication factors of conventional calculations without considering thermal agitation and those calculated by (2) for considering thermal agitation.

The technique shown in this section is useful to obtain breakdown in isotopes, reaction types, and energy group because each of the parameters is evaluated separately.

3.2. Calculation Results. The impact on Doppler coefficient is summarized in Table 3. Table 3 shows that the impact on Doppler coefficient is small at high Gd_2O_3 concentration and the impact is enhanced at low Gd_2O_3 concentration, as also shown in Table 2 where the results were obtained by Monte Carlo calculations. There are some differences in magnitude between Tables 2 and 3, but the tendency of the impact

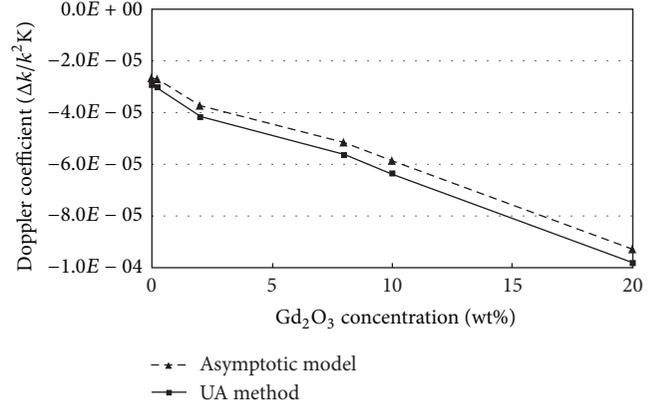


FIGURE 2: Comparison of Doppler coefficient.

is the same. Therefore further considerations were carried out to reveal the mechanism of the tendency especially to reveal the factor to cause the enhanced impact at low Gd_2O_3 concentration.

Doppler coefficients calculated by conventional asymptotic kernel model and UA method are shown in Figure 2. Figure 2 shows that the magnitude of Doppler coefficient becomes large monotonically and linearly according to the increment of Gd_2O_3 concentration.

Table 4 presents the nuclide and reaction breakdown of the impact on Doppler coefficient. Another breakdown by energy range is summarized in Table 5. As shown in Tables 4 and 5, U-238 capture reaction is the dominant cause of the impact of thermal agitation on Doppler coefficient, and the impact is remarkable at the energy around 21, 37, and 66 eV as already reported in the literature [2–5]. In addition to this, the impact of thermal agitation on Doppler coefficient depends on Gd_2O_3 concentration and the impact increases at low Gd_2O_3 concentration compared to pure UO_2 fuel as shown in Tables 4 and 5.

4. Discussions

The impact of thermal agitation on Doppler coefficient increases up to about 12% when Gd_2O_3 concentration is around 0.2 wt% and 2 wt% and the impact decreases according to the increment of Gd_2O_3 concentration although Gd isotopes do not have the impact of thermal agitation on Doppler coefficient as shown in Table 4.

In order to discuss this tendency, a simplified expression of the difference in Doppler coefficient is derived in Section 4.1 for detailed consideration of the mechanism. Section 4.2 shows the numerical results by using the simplified expression and the discussion of the mechanism especially to cause the enhanced impact at low Gd_2O_3 concentration.

4.1. Derivation of Simplified Expression. In this section, the impact on Doppler coefficient ($\Delta D.C$) caused by thermal agitation is expressed in simple expression for easy consideration to reveal the mechanism.

TABLE 4: Nuclide and reaction breakdown of impact on the Doppler coefficient of Gd-bearing fuel.

Nuclide reaction	Gd ₂ O ₃ concentration [wt%]					
	0	0.2	2	5	10	20
U-238 capture	9.4%	12.2%	12.0%	10.6%	8.4%	5.4%
U-235 capture	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Gd-155 capture	—	0.0%	0.0%	0.0%	0.0%	0.0%
Gd-156 capture	—	0.0%	0.0%	0.0%	0.0%	0.1%
Gd-157 capture	—	0.0%	0.0%	0.0%	0.1%	0.1%
Gd-158 capture	—	0.0%	0.0%	0.0%	0.0%	0.0%
All	9.4%	12.2%	12.0%	10.6%	8.5%	5.6%

TABLE 5: Energy breakdown of impact on the Doppler coefficient of Gd-bearing fuel.

Energy range [eV]	Gd ₂ O ₃ concentration [wt%]					
	0	0.2	2	5	10	20
3.93~5.04	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5.04~6.48	-0.1%	-0.2%	-0.1%	-0.1%	-0.1%	0.0%
6.48~8.32	0.9%	1.1%	0.8%	0.7%	0.4%	0.2%
8.32~10.68	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
10.68~13.71	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
13.71~17.60	0.0%	0.0%	0.0%	0.0%	0.1%	0.1%
17.60~22.60	2.1%	2.7%	2.6%	2.2%	1.7%	1.0%
22.60~29.02	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
29.02~37.27	4.6%	6.1%	6.2%	5.6%	4.6%	3.1%
37.27~47.85	-0.2%	-0.2%	-0.2%	-0.2%	-0.2%	-0.1%
47.85~61.44	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
61.44~78.89	1.4%	1.8%	1.8%	1.6%	1.3%	0.8%
78.89~101.3	0.0%	-0.1%	0.0%	0.0%	0.0%	0.0%
101.3~130.1	0.7%	1.0%	0.9%	0.8%	0.7%	0.5%
All	9.4%	12.2%	12.0%	10.6%	8.5%	5.6%

The impact of Doppler coefficient by thermal agitation at energy group g only is expressed as

$$\begin{aligned} \Delta D.C^g &= \frac{\{(1/k_{low,UA}^g - 1/k_{high,UA}^g) - (1/k_{low,conv} - 1/k_{high,conv})\}}{\Delta T} \\ &= \frac{\{((k_{low,conv} - k_{low,UA}^g)/k_{low,UA}^g k_{low,conv}) - ((k_{high,conv} - k_{high,UA}^g)/k_{high,UA}^g k_{high,conv})\}}{\Delta T}, \end{aligned} \quad (4)$$

where k_{UA}^g is a multiplication factor which treats thermal agitation effect at energy group g and calculated by $k_{UA}^g = k_{conv} \cdot (1 + d^g \cdot S^g)$ as easily expected from (2). Therefore, (4) can be transformed as

$$\begin{aligned} \Delta D.C^g &= \frac{\{(-d_{low}^g S_{low}^g / k_{low,UA}^g) - (-d_{high}^g S_{high}^g / k_{high,UA}^g)\}}{\Delta T}. \end{aligned} \quad (5)$$

The change of S^g by the change of temperature is not remarkable compared to the other parameters as shown in

later sections (Figure 4). Thus, the sensitivity coefficient can be approximated as

$$S^g \cong S_{low}^g \cong S_{high}^g. \quad (6)$$

Then, (5) can be transformed as

$$\Delta D.C^g \cong \frac{S^g (d_{high}^g / k_{high,UA}^g - d_{low}^g / k_{low,UA}^g)}{\Delta T}. \quad (7)$$

For further simplification of (7), following approximations are considered.

The capture cross section of Gd nuclide is remarkably large at thermal range, but the magnitude is not so large

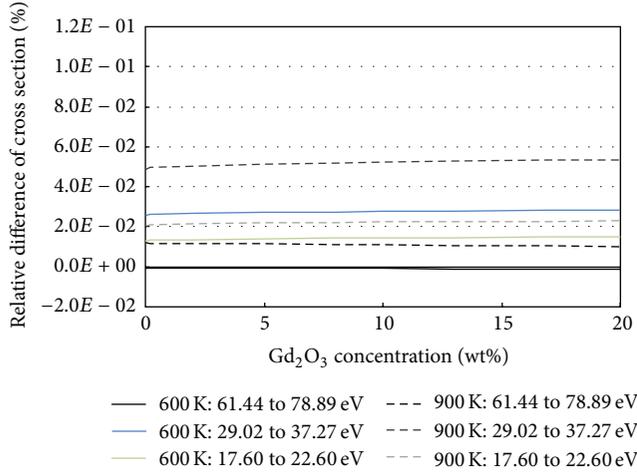


FIGURE 3: Relative difference of U-238 capture cross section.

compared to that of U-238 at the energy group where the agitation effect is sensitive to Doppler coefficient. Thus, d^g of U-238 does not strongly depend on Gd_2O_3 concentration at the energy group and the difference of d^g is nearly independent of Gd_2O_3 concentration as shown in Figure 3. Therefore, new parameter A^g can be set as independent parameter of Gd_2O_3 concentration as

$$A^g \cong d_{high}^g - d_{low}^g. \quad (8)$$

By using (8), (7) is transformed as

$$\begin{aligned} \Delta D.C^g &\cong \frac{S^g ((A^g + d_{low}^g)/k_{high,UA}^g - d_{low}^g/k_{low,UA}^g)}{\Delta T} \\ &= \frac{S^g ((d_{low}^g (k_{low,UA}^g - k_{high,UA}^g) + A^g k_{low,UA}^g)/k_{high,UA}^g k_{low,UA}^g)}{\Delta T}. \end{aligned} \quad (9)$$

Practically, $(k_{high,UA}^g - k_{low,UA}^g)$ is quite small compared to $k_{low,UA}^g$ in the evaluation of the difference in Doppler coefficient. Therefore, (9) can be simplified by neglecting $(k_{high,UA}^g - k_{low,UA}^g)$ to obtain

$$\Delta D.C^g \cong \frac{A^g (S^g/k_{high,UA}^g)}{\Delta T}. \quad (10)$$

Equation (10) shows that the difference in Doppler coefficient as a function of Gd_2O_3 concentration can be simply discussed as the product of the sensitivity coefficient and the inverse of multiplication factor.

4.2. Impact on Doppler Coefficient. In this section, the impact of thermal agitation on Doppler coefficient in epithermal range is discussed by using (10). The sensitivity coefficient S^g of U-238 capture cross section to multiplication factor is shown in Figure 4. Figure 4 shows that the magnitude of S^g decreases according to the increment of Gd_2O_3 concentration since the ratio of the capture reaction of U-238 to total capture rate becomes small according to the increment of Gd_2O_3

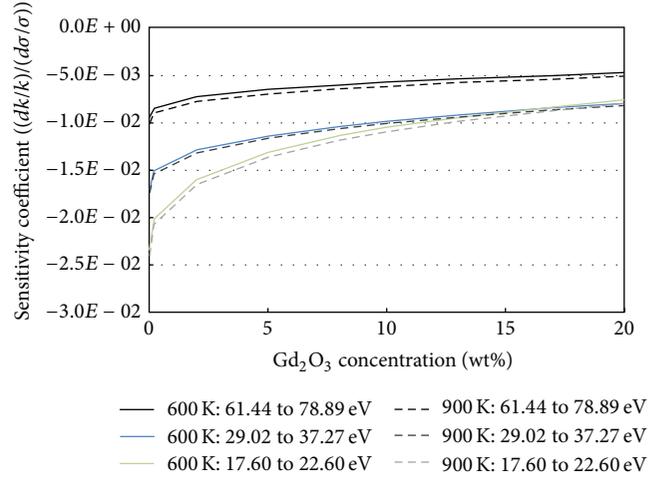


FIGURE 4: Sensitivity coefficient of U-238 capture cross section to multiplication factor.

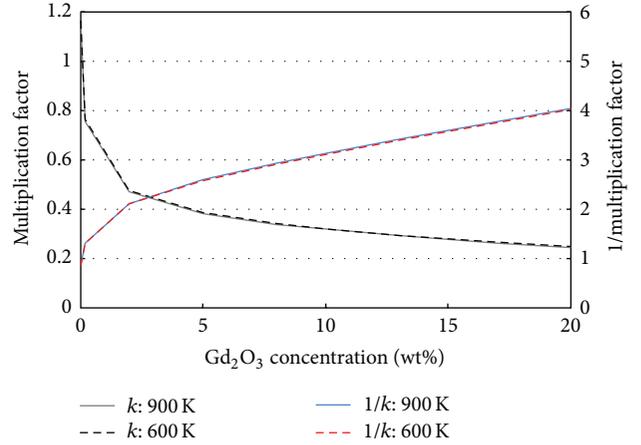


FIGURE 5: Multiplication factor and inverse of multiplication factor.

concentration. Figure 5 shows the multiplication factor and the inverse of the multiplication factor as a function of Gd_2O_3 concentration. Figure 5 shows that the inverse of multiplication factor increases monotonically by adding Gd_2O_3 because of its huge capture cross section. Figure 6 shows the difference in Doppler coefficient evaluated by exact solution and the simplified expression expressed as (10). Two evaluations shown in Figure 6 are almost the same, which shows the correctness of the simplified expression. Particular behavior of the impact as a function of Gd_2O_3 concentration can be interpreted by using the above mentioned results as follows.

As already described, there is a maximum impact of thermal agitation on Doppler coefficient at low Gd_2O_3 concentration and this tendency comes from the rapid increase of $1/k$ and slow increase of the magnitude of Doppler coefficient at low Gd_2O_3 concentration as shown in Figures 2 and 5. In other words, the sensitivity coefficient in Figure 4 shows the decrement in magnitude according to the increment of Gd_2O_3 concentration because of the increment of Gd_2O_3

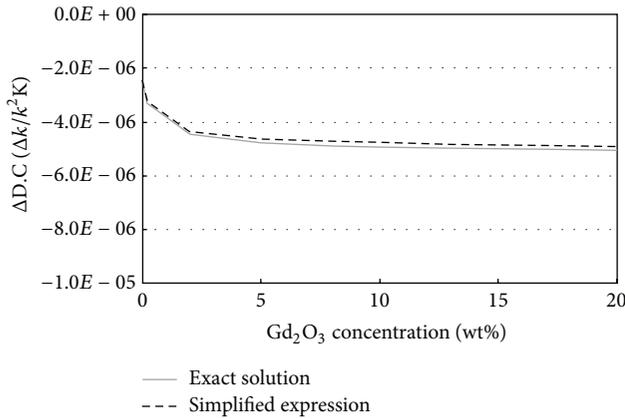


FIGURE 6: Difference in Doppler coefficient.

capture rate to total capture rate; on the other hand, the decrement of multiplication factor is remarkable especially at low Gd_2O_3 concentration as shown in Figure 5. And at high Gd_2O_3 concentration, the value of $\Delta D.C./D.C$ becomes small and is mainly caused by the fact that the magnitude of Doppler coefficient becomes huge although $\Delta D.C$ is almost constant as shown in Figures 2 and 6. This is the reason why there is a maximum point of the impact on Doppler coefficient for Gd-bearing fuel.

Similar tendency which shows a maximum impact is expected for the fuel with the slight content of strong absorber. Therefore, Doppler coefficient of the system which contains low content of strong absorber should be analyzed carefully with the consideration of thermal agitation.

5. Conclusions

The impact of thermal agitation on Doppler coefficient of Gd-bearing fuel was analyzed. The results show that the impact increases by adding a small amount of Gd_2O_3 (~2 wt%) to UO_2 fuel, although the impact decreases by adding a large amount of Gd_2O_3 (~10 wt%) to UO_2 fuel. This tendency was analyzed with the usage of simplified expression of the difference in Doppler coefficient. The difference in Doppler coefficient varies as a function of Gd_2O_3 concentration, and this is mainly caused by the two factors: sensitivity coefficient of U-238 capture cross section to multiplication factor and multiplication factor. The magnitude of both factors decreases according to the increment of Gd_2O_3 concentration, but the decrement rate of multiplication factor is remarkable compared to that of the sensitivity coefficient at low Gd_2O_3 concentration, where the self-shielding of Gd isotopes is not so important and the content of U-238 is roughly the same to the fuel without Gd_2O_3 . The decrement rates of both factors are almost the same at high Gd_2O_3 concentration, which brings almost the same difference in Doppler coefficient between with and without considering thermal agitation. On the other hand, the magnitude of Doppler coefficient increases monotonically and linearly according to the increment of

Gd_2O_3 , mainly caused by the decrement of multiplication factor. Therefore, there is a maximum point of the relative difference in Doppler coefficient caused by thermal agitation.

Similar tendency is expected for other strong-absorber-bearing fuel. Thus, it should be noted that the Doppler coefficient of the fuel with a slight amount of strong absorber should be analyzed carefully with the consideration of thermal agitation.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

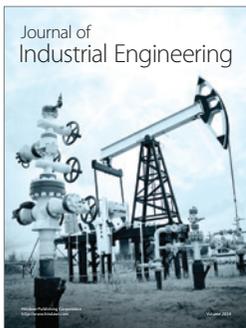
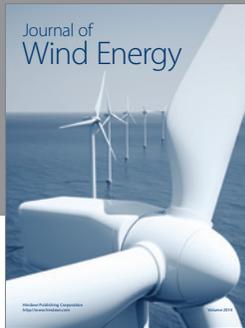
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