Dynamic simulation of VIP moisture and heat transport

Beck, A.; Binder, M.; Frank, O.
Stuttgart University of Applied Sciences
Schellingstr. 24, 70147 Stuttgart
E-Mail: Andreas.Beck@hft-stuttgart.de

Theme 4: VIP Performance – Optimisation, Testing, and Modeling

Keywords: Simulation, moisture transport, moisture disposition, transient measurement

Abstract

The coincidence of high temperatures and high relative humidities can cause damage to the silica core of a Vacuum Insulation Panel (VIP) as well as to its envelope. To evaluate to what extent these unfavourable conditions occur within VIPs integrated in different building elements a simulation tool was developed. It calculates heat and moisture transport simultaneously. The physical model underlying the calculation tool takes into account two mechanisms of water transport in the VIP: Knudsen diffusion and surface diffusion, the latter describing the random hopping of molecules on the silica surface. The transport coefficients which are crucial for depicting the transport processes realistically were determined by transient heat flow measurements.

The hygrothermal conditions computed for typical plastered VIP constructions were consistently moderate and thus according to the current state of knowledge not destructive. Different types of VIP applications can be evaluated in future calculations. Further experimental research on the effects of moisture on VIPs is recommended in oder to deduce palpable predictions of long term behaviour from the calculation results.

1. INTRODUCTION

In recent years VIP have found their way into the building sector in Germany far beyond the early pilot projects. As different possibilities of application have been tested intensely and consequently various products have been awarded general technical approval, further wide-spread use of the technology can be foreseen.

Becoming a mass market product, however, questions of the aging behavior of VIPs gain importance as long term service of the panels has to be guaranteed. Especially the influence of water vapor infiltrating the VIPs over the years and the resulting moisture content of the kernel material is not determined conclusively. Various tests showed that the silica core (Morel et al, 2007) as well as the envelope (Brunner et al, 2008) can be damaged by disadvantageous combinations of high temperatures and high moisture content.

The hygrothermal conditions which occur within a VIP depend on the instationary thermal boundary conditions it is exposed to. As far as building applications are concerned, these are mainly defined by the composition of the respective structural element and its orientation. To classify different typical applications with regard to risks to the VIP a simulation model has to be developed which comprehends heat and moisture transport.

2. THEORY

To explain the moisture transport within a VIP two mechanisms are considered.

a) Knudsen diffusion

If the diameters of the pores are of the same order of size as the mean free path of the molecules, the transport is governed by molecule-wall collisions. In this case the diffusion coefficient is given by (Krishna et al, 1997)

$$D_K = \frac{\phi}{\tau_K} \frac{d}{3} \sqrt{\frac{8RT}{\pi M}} \qquad (1)$$

where d is the pore diameter. The square-root represents the mean molecular velocity (R: ideal gas constant, T: Temperature, M: molar mass). Φ is the porosity and τ_K the tortuosity factor which takes into account the morphology of the VIP, i.e. the pore geometry and the connectivity of the pore network. For a cylindrical pore $\tau_K = 1$.

b) Surface diffusion

To describe the surface migration of adsorbed water molecules the random hopping model (Higashi et al, 1963) was used. The random hopping model views surface diffusion as a flow due to a number density gradient on the surface. An adsorbed molecule has to overcome an energy barrier E_{act} to jump to the next vacant site on the surface. Thereby the residence time τ till the molecule jumps is given by

$$\tau = \frac{1}{v} e^{E_{act}/RT} \qquad (2)$$

E_{act} is the activation energy of migration and v the vibration frequency of the bond holding the molecule to the site.

Regarding the surface flow as a random walk the surface diffusion coefficient $D_{s,o}$ is obtained by Einstein's equation (Yang et al, 1973)

$$D_{s,o} = \frac{l^2}{2\tau} \qquad (3)$$

where l is the average distance between two sites. To take into account the situation of occupied sites the total diffusion coefficient is given by

$$D_s = \frac{D_{s,o}}{\tau_S} \frac{1}{1-\theta} \qquad (4)$$

θ is the surface coverage and τ_S is the tortuosity factor of the silica surface.

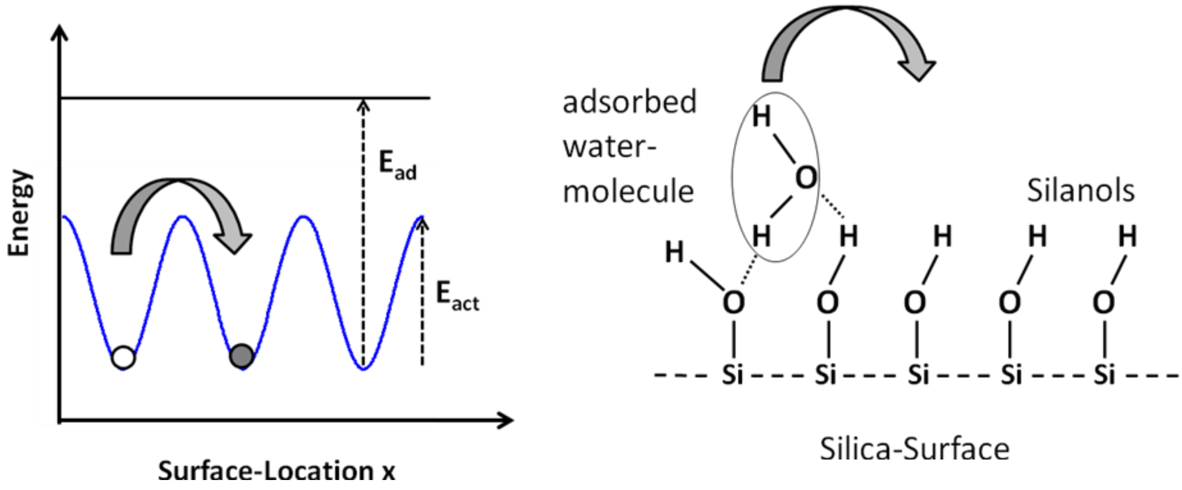


Figure 1: Schematic view of the energy structure on the silica surface (left). Silica surface chemistry (right). Both are showing the molecule hopping process.

By incorporating both mechanisms into the coupled heat and moisture transport equations in (Beck et al, 2007) we get

$$\varrho \frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left\{\frac{D_K}{RT}\frac{\partial p}{\partial x} + D_s \frac{\partial n_s}{\partial x}\right\} \quad (5)$$

$$\varrho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left\{\lambda(p)\frac{\partial T}{\partial x} + E_{ad}\frac{D_K}{RT}\frac{\partial p}{\partial x}\right\} \quad (6)$$

Equation (5) describes the moisture transport due to the partial pressure (p) gradient of the local moisture content and to the gradient of the surface density n_s of the adsorbed water molecules. n_S = f(p) depends on the local pressure and on the sorption isotherm described in (Heinemann, 2008). Equation (6) describes the heat transport due to the thermal conductivity as well as due to the enthalpy transport (second term), respectively.

ρ is the mass density of the VIP, u the water content referred to the skeleton mass of the SiO_2-network, c_p the heat capacity, λ(p) the pressure dependent thermal conductivity and E_{ad} the heat of adsorption.

3. MEASUREMENT AND ANALYSIS

In order to determine the transport coefficients the model described above was used to analyze the measurements presented in (Beck et al, 2007). From the temperature dependency of λ of a VIP with a moisture content of 4.2 %-mass a value for the activation energy for surface migration E_{act} = (20 ± 2) kJ/mol was obtained. E_{act} represents nearly half of the adsorption enthalpy of a monolayer of water on the silica surface.

Fitting the λ(u)-measurements presented in (Beck et al, 2007) with the model described above a surface diffusion coefficient of

$$D_{s,0}/\tau_s = (3.0 \pm 0.3) \cdot 10^{-10}\, m^2/s$$

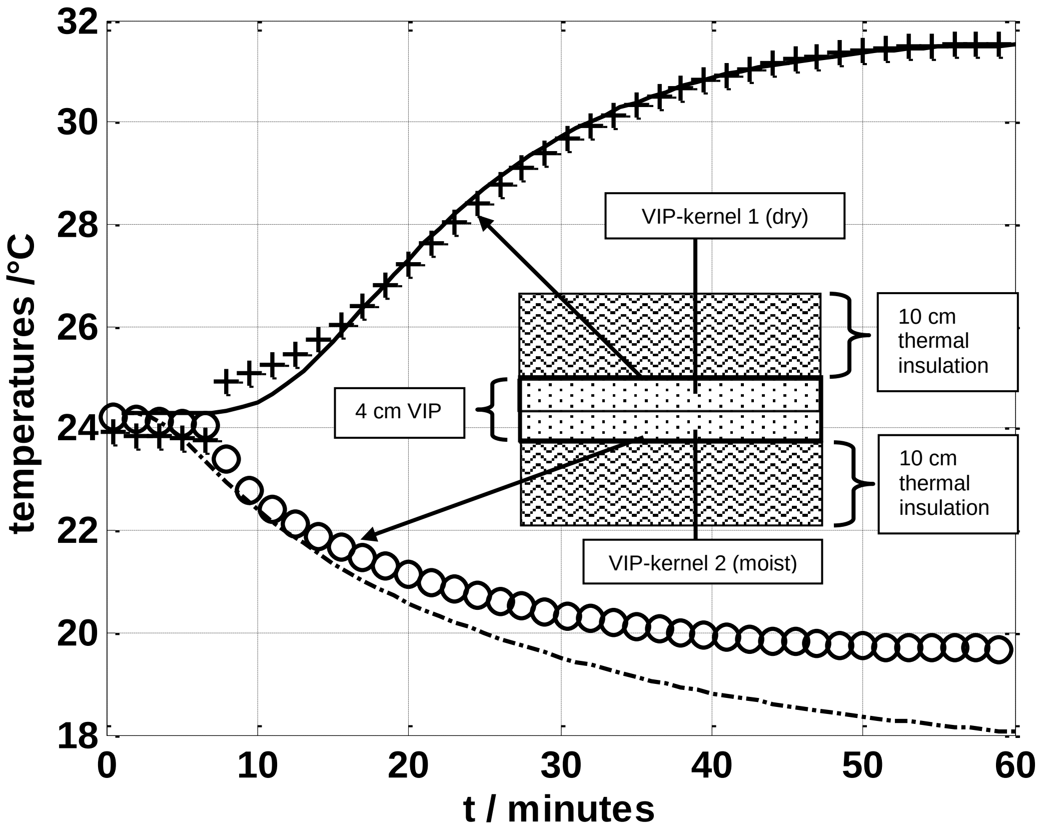
was calculated for room temperature. To determine τ_S we used measurement data of (Clark et al, 1985) where a residence time of $\tau = 6 \cdot 10^{-11} s$ was obtained via neutron scattering and an OH surface concentration of 4.6 nm^{-2} was given. The last yields a minimum distance between two absorbed water molecules of l = 0.53 nm. Using these results a diffusion coefficient of $D_{s,o} = l^2/2\tau \approx 2 \cdot 10^{-9}\, m^2/s$ for a SiO_2-surface was obtained. Combining this value with the diffusion coefficient obtained via thermal measurements (λ(u)) a tortuosity factor of $\tau_s = 8 \pm 1$ was calculated.

The calculated surface diffusion coefficient is obtained under the assumption that the total increase in the thermal conductivity is caused by moisture by surface migration and water vapor pressure. An increase of λ due to shortening of contact points of the various clusters is not considered. Three arguments are against this assumption:

a) No strong increase of the sorption isotherm at small humidity was detected. An increase which can be responsible for filling small capillary regions is firstly observed above humidity's of φ = 70 %.
b) The SiO_2-network is completely covered with water molecules above a water content of 10 mass-%. The accumulation of water molecules at special points requires very small radian of curvature.
c) The temperature dependence of the thermal conductivity cannot be explained strong by increase of a temperature dependence of the contact resistances.

To determine the Knudsen diffusion coefficient we performed transient heat flow measurements. For this purpose a special VIP was constructed. It was composed of a dry and a moist (2.68 mass-%) silica kernel, each of them 2 cm thick. After evacuation moisture disposition by gas diffusion takes place within the VIP. This causes temperature changes on the surfaces of the VIP due to the desorption and adsorption of moisture.

To register the time dependent temperatures on the VIP it was integrated between two layers of conventional thermal insulation (thickness 10 cm). The system of measurement is shown in Figure 2. After 58 minutes the measurement was stopped and the moisture redistribution which had happened until then was determined by weighing the two kernel parts. This way two parameters were known to determine the necessary transport coefficients and test the simulation model.



+++++ measured temperature dry kernel [°C]

ooooo measured temperature moist kernel [°C]

……… simulated temperature dry and moist kernel [°C]

moisture diposition after measurement

	Measured	simulated
kernel 1	1.94 mass-%	2.0 mass-%
kernel 2	0.81 mass-%	0.7 mass-%

Figure 2: Time dependent temperatures measured on the surface of a VIP composed of a dry and a moist silica kernel. The lines show the best fitted temperatures gained via simulation.

Using the coupled differential equations (5) and (6) together with a heat of adsorption of $E_{ad} = 50\ kJ/mol$ (water – silica) a diffusion coefficient of

$$D_K = (1.6 \pm 0.2) \cdot 10^{-5}\ m^2/s$$

fits well. Via equation (1) and a porosity of 90% a value of $d/\tau_K = (92 \pm 10)\ nm$ was found which agrees with poresize measurements obtained via thermal conductivity measurements (Fricke et al, 2007).

4. PREDICTION AND DISCUSSION FOR VIP-APPLICATIONS IN BUILDINGS

As described in (Morel et al, 2007), a coincidence of high temperatures and high relative humidity reduces the specific surface area of pyrogenic silica. Since the nano-structured character of the silica network is mainly responsible for its extremely low solid thermal conductivity, this moisture induced aggregation causes permanent degradation of a Vacuum Insulation Panel.

How strongly a VIP is affected by these unwanted effects depends on the transient thermal boundary conditions it is exposed to. As far as building applications are concerned, these are mainly defined by the composition of the respective structural element and its orientation.

Using the transport coefficients determined experimentally the theoretical model presented above allows for the prediction of the hygrothermal conditions (relative humidity, temperatures) which occur within VIPs in building applications. Thus typical constructions can be classified with regard to the frequency of occurrence of unfavourable situations which bear the risk of structural damages to the silica skeleton.

For this paper two different constructions have been examined that way, both of them composed of a massive brick wall coated on the outside with VIPs. Construction # 1 adds another layer of conventional insulation material as a plaster base whereas in construction # 2 plaster is applied directly on the VIP. The material data of both constructions are compiled in table 1.

				Construction #1	Construction #2
Material	Heat capacity [kJ/(kg*K)]	Thermal conductivity [W/(m*K)]	Density [kg/m³]	Thickness of layer [m]	Thickness of layer [m]
Brick	1000	0.5	2000	0.30	0.30
VIP	700	Variable	200	0.02	0.02
Additional insulation	1000	0.04	30	0.00	0.02
Plaster	1000	0.8	1000	0.005	0.005

table 1: Material data of the examined wall constructions

The simulation was carried out with an initial moisture content of 3 mass-%, referring to the mass of the dry silica core. According to the sorption isotherm this corresponds to a relative humidity of about 50%

To represent realistic conditions in the simulation the outside temperature and solar irradiation were taken from test reference year data for the location of Wuerzburg / Germany. The room temperature was set to 20 °C constantly.

As the temperature of the outside of the VIP depends strongly on the solar irradiation absorbed by the plaster layer, comparative simulations with different orientations of the wall and absorption coefficients were made.

Extreme conditions within the VIP are expected to occur at the borders of the system, e.g. either at the enclosure orientated towards the room (interior) or at the one facing to the outside (exterior). For that reason these positions were evaluated. The results are plotted in Figure 3 - 4.

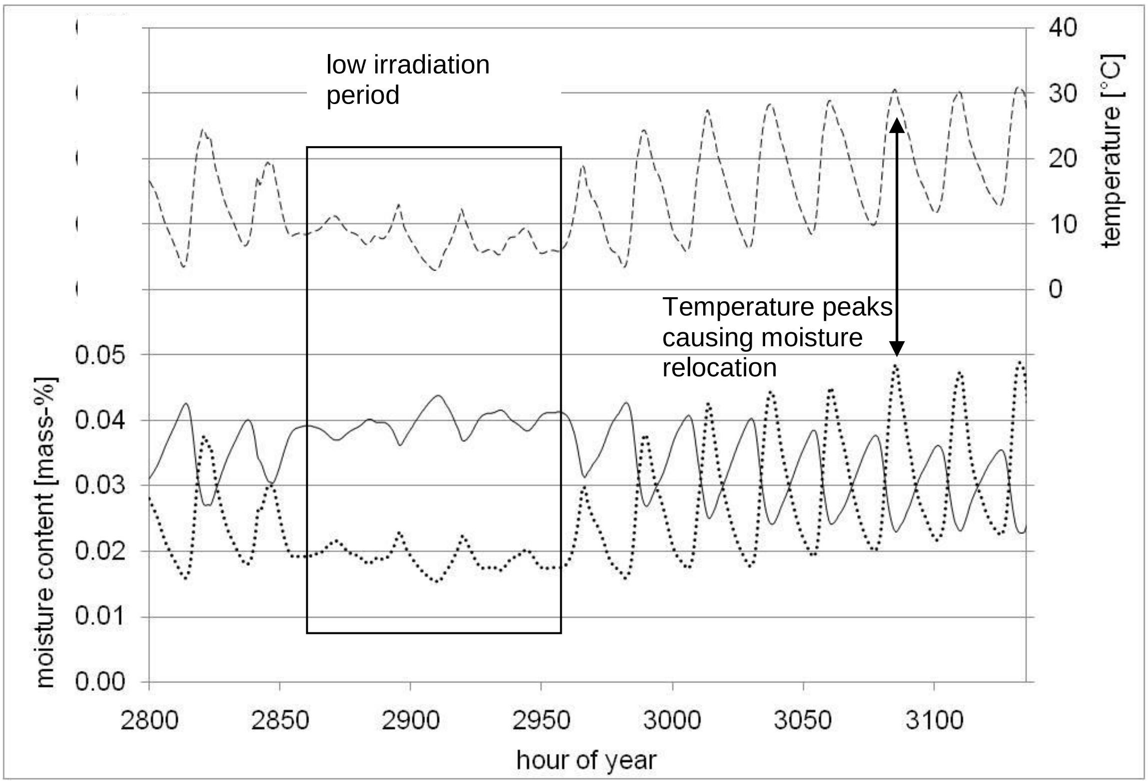


Figure 3: Hygrothermal conditions within a VIP as calculated with the model described above: temperature on the outward facing side of the VIP (- - -); mass related moisture content on the outward (——) and inward facing side (···). The graph refers to a southward orientated wall composed according to table 1, construction type #1.

Figure 3 exemplifies the results gained directly out of the simulation. It shows the hygrothermal conditions within a VIP during a two week period in April / May. The examined VIP is integrated in a southward orientated wall composed according to the description of table 1, construction #1.

The figure depicts two different environmental situations and their impact on the processes of moisture distribution within the panel. During the first week due to cloudy weather low irradiation impinges on the wall. The temperature on the outside of the VIP remains within a narrow band. Congruously the moisture distribution does not change significantly either. In the second week stronger solar irradiation leads to increased temperature fluctuations on the outside of the VIP with peaks around noon. Consequently water is driven out of regions near to the surface towards the back side of the panel, leading to moisture peaks there. During nighttime the reverse process is taking place.

By simulating a whole annual cycle the hygrothermal states occurring in the VIP during a year can be determined. For the two construction types described in table 1 they are plotted in Figure 4.

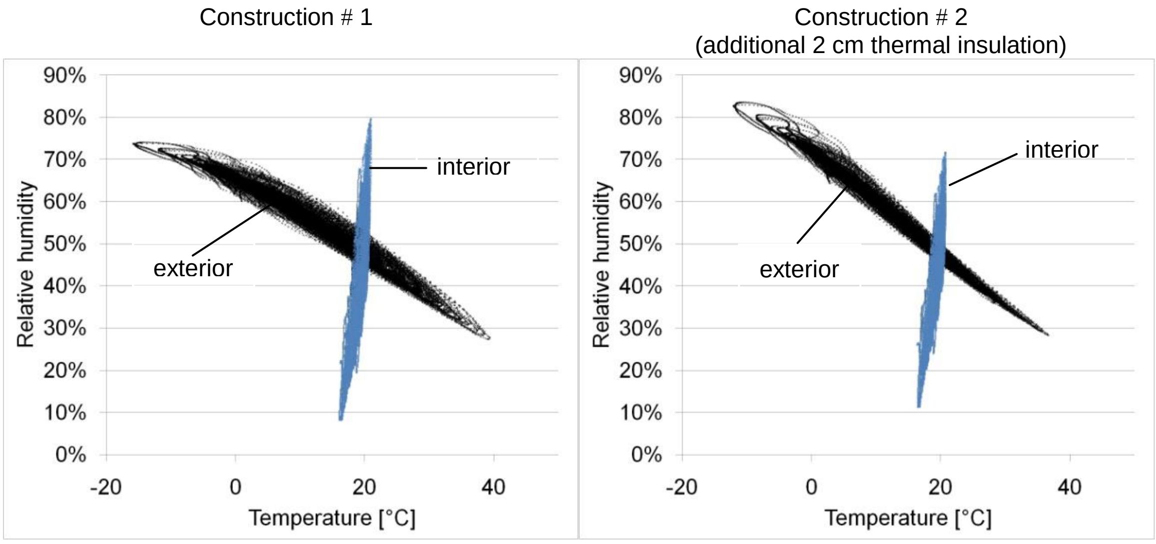


Figure 4: Hygrothermal states (temperature / relative humidity) occurring at the interior and exterior boundary of the VIP during an annual cycle. Each point in the graph represents a ten minute simulation step. Wall constructions according to table 1; solar absorption coefficient of the plaster layer a = 20%. Both walls were assumed south orientated.

The diagrams show that high relative humidities of > 70% do appear both near the exterior and the interior boundary of the VIP; however they always go along with temperatures < 20°C. According to (Morel et al, 2007) no decrease of the silica's specific surface area has to be expected under these conditions.

Higher temperatures around 40°C are only reached on the outside of the VIP but due to the moisture transport processes described above they coincide with low relative humidities. This is also true for constructions with darker plaster layers with a solar absorption coefficient of 70% where temperatures up to 60 °C can arise.

The additional thermal insulation taken into account in the diagram on the right reduces the impact of solar irradiation on the VIP and thus the amount of water transported to its back side. Consequently the maxima of relative humidity are displaced from the back side to the front side of the VIP.

5. OUTLOOK AND CONCLUSION

By using the simulation model with the transport coefficients found experimentally it is possible to calculate the dynamic moisture disposition and redistribution in the kernel of a VIP and its temperature profile simultaneously. This way different types of constructions can be compared. The risk of damages to the silica structure due to unfavoured hygrothermal conditions can be estimated e.g. by resorting to publications mentioned in this paper. As these primarily dealt with extreme conditions further research referring to situations that are more probable in real building applications is advisable.

Bibliography

BECK, A., BINDER, M. and FRANK, O. Influence of water content on the thermal conductivity of vacuum panels with fumed silica kernels, IVIS 2007

BRUNNER, S., SIMMLER, H. and WAKILI, K.G. Vakuumisolation – Materialspezifische Aspekte bei der Alterung, *15. Schweizerisches Status-Seminar „Energie- und Umweltforschung im Bauwesen“,* Zürich 2008

CLARK, J.W., HALL, P.G., PIDDUCK, A.J. and WRIGHT, C.J. Molecular Diffusion in Monolayer Films of Water Adsorbed on a Silica Surface, *J. Chem. Soc., Faraday Trans., 1985, **81**, pp.2067-2082*

FRICKE, J. BECK, A. and BINDER, M. Vakuum-Isolationspaneele für Gebäude, *ISBN 978-3-00-022618-2, 2007*

HEINEMANN, U. Influence of Water on the Total Heat Transport in Evacuated Insulations, *Int. J. Thermophya*., DOI 10.1007/10765-007-0361-1, Springer Science+Business Media, LLC 2008

HIGASHI, K., ITO, H. and OISHI, I. Surface diffusion phenomena in gaseous diffusion, *J. Atomic Energy Society Japan*, 5, 846, 1963

KRISHNA, R. and WESSELINGH, J.A. The Maxwell-Stefan approach to mass transfer, *Chem. Eng. Science*, **52**, 6, 1997, pp. 861-911

MOREL, B., AUTISSIER, L., AUTISSIER, D. et al. Modifications of a pyrogenic silica exposed to moist air, IVIS 2007

YANG, R.T., FENN, J.B. and HALLER, G.L. Modification to the Higashi Model for surface diffusion, *AIChE Journal*, 19, 1973, p.1052