Gas Quality Tracking in distribution grids with SmartSim –
a new kernel for flow calculation

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Abstract

This article presents a novel calculation kernel for the simulation of gas distribution grids. The kernel is characterized by a high degree of accuracy and extremely short calculation times. By fully integrating the new kernel into the SmartSim software for CV tracking complex grids can be calculated very efficiently. For the first time an uncertainty evaluation of the calculated CVs for all exit points of a gas grid is carried out based on a Monte Carlo Simulation according to the Guide to the Expression of Uncertainty in Measurement (GUM). Experimental results are derived from a regional distribution grid of Avacon and presented in this paper.

1 Introduction

National gas markets growing together to form a European gas market and rising imports of liquefied natural gas (LNG) transported to Europe by tanker have led to wider variations in gas quality and thus in calorific values (CVs) over the past few years. This trend has been reinforced by an increasing production of bio methane, which is injected into distribution grids. Before injection bio methane is usually conditioned to obtain the CV prevailing in the grid in order to match the required accuracy in billing. In group-H gas areas this is achieved by admixing propane.

In Germany gas quality tracking systems have been used in transmission grids for some years now and are state-of-the-art technology [1]. Such systems allow the CV to be calculated for any point in the grid at any time. The necessary input parameters include verified measured values for the CV at the entry points and the respective entry and exit volumes. German verification regulations [2] require the CVs at end users to be de-

termined with an uncertainty not exceeding 2 % (the maximum permissible error in billing).

In distribution grids, volumes at exit points are often not measured, so the SmartSim method has been developed by E.ON Technologies as a gas quality tracking system for these grids. This method determines the exit volumes from so-called standard load profiles (SLP) in combination with a new correction algorithm. The method was approved in August 2012 by the German authorities for legal metrology. Where SmartSim is used therefore, cost-intensive admixing of propane in connection with bio methane injection will no longer be necessary and the economics of biogas plants can be improved. The method has been described previously in gas for energy 3/2012 [3].

2 Gas Quality Tracking with SmartSim

SmartSim requires topological data and measured values as input parameters. The topological data include the length, diameter and roughness of the pipes. The hourly measurements are the CVs measured at the entry points and the entry and exit volumes. Because exit volumes are not usually measured in distribution grids, they are estimated using standard load profiles (SLPs) developed at Technical University of Munich [4] including customer-specific consumption data. In order to reduce uncertainties of estimates for SLP-volumes an appropriate volume balance of the grid is performed in SmartSim. Beside the entry and exit volumes, the linepack ΔV_{grid} is also taken into account.

$$V_{corr} = V_{en} - V_{SLP} - V_{meas} - \Delta V_{grid} \qquad (1)$$

The correction volume V_{corr} obtained with Eq. (1) is split among the individual SLP consumers using Eq. (2). In this manner, the adherence of the grid's volume balance can be guaranteed at any point and any time.

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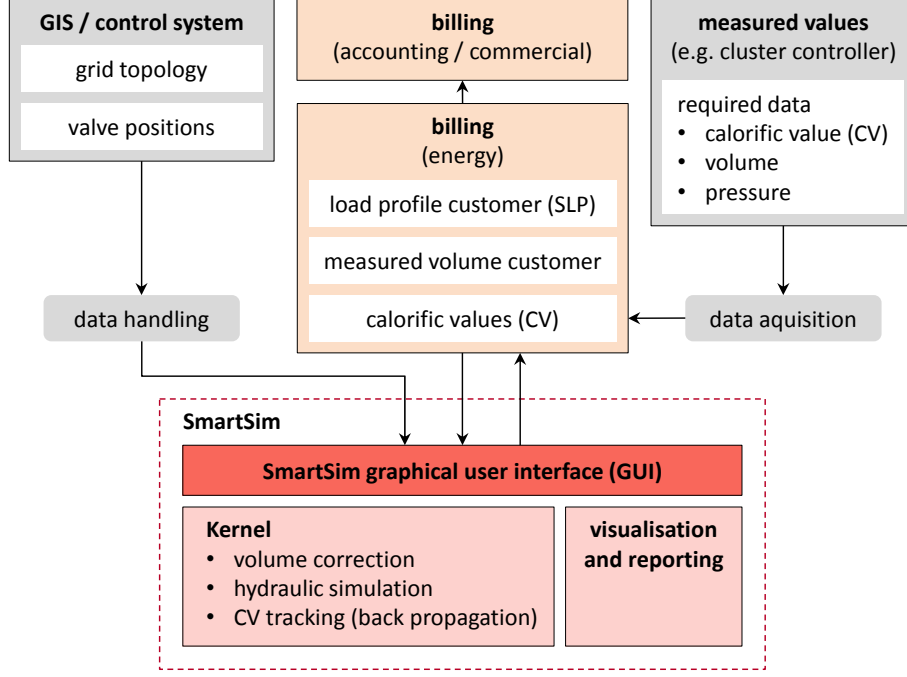[3] University of applied sciences Munich

Figure 1 SmartSim Input Parameters.

$$\widehat{V}_{\text{SLP},i} = \left(1 - \frac{V_{\text{corr}}}{\sum_j V_{\text{SLP},j}}\right) \cdot V_{\text{SLP},i} \qquad (2)$$

Put simply, the method is carried out in the following three steps, see SmartSim Kernel in Figure 1:

1. volume correction
2. hydraulic simulation
3. CV tracking (back propagation)

Once the volumes for each hour have been corrected using Eq. (2), the grid's flow situation is determined by a hydraulic calculation. Afterwards the flow velocities as well as the mass and volume flow rates in the individual pipes are known now. In the final step, for every exit point the exit volumes are tracked back through the grid until reaching the entry points. This is done with the help of a special gas package model, the so-called 'back-propagation algorithm'. This algorithm enables SmartSim to determine the proportions of the injected gases at each exit point, including information on the time the gas is transported through the grid. The advantage of this approach is that any exit value can always be related to the verified entry value. A further benefit is that other relevant gas characteristics such as the K number or CO_2 emission factor can be derived from the entry points in a single calculation step. As a result, SmartSim supplies calorific values for all exit points in the grid, which can then be used for billing. The billing CV is usually determined as the volume-weighted monthly average value.

3 DEVELOPMENT OF AN INTEGRATED KERNEL FOR SMARTSIM

Compared with transportation grids, regional distribution grids usually have more complex grid structures, lower flow velocities and lower gas pressures. This is why the present study initiated the development of a kernel that has been optimised specifically to meet these requirements. Incorporating flow simulation into SmartSim also offers greater flexibility in terms of handling and interfacing with other IT systems.

A complete description of the flow situation is based on the three conservation equations of mass, pulse and energy. Pulse and energy conservation is used to describe dynamic changes of state such as pressure surges, which propagate inside the gas grid at the speed of sound within a few seconds or minutes (as the overall grid length is in the order of 10 to 100 kilometres). Since the temporal resolution of the input data is usually one hour, the influence of dynamic state changes that are described by pulse and energy conservation can therefore be neglected. The hydraulic calculation hence simplifies to the mass conservation equation:

$$\left(\frac{\partial(\rho A)}{\partial t}\right)_x + \left(\frac{\partial(u\rho A)}{\partial x}\right)_t = 0 \qquad (3)$$

When simulating pressure changes in the gas grid, the temporal derivation is not equal to zero. These pressure fluctuations are due to differences in the injected and offtaken gas mass, the

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so-called linepack. The following mass balance is calculated hourly for the whole natural gas grid to determine the pressure change within the grid:

$$\Delta m = \sum m_{\mathrm{E}} - \sum m_{\mathrm{A}} \qquad (4)$$

The difference Δm is split among the individual pipes taking the pressure distribution in the gas grid into consideration. The mass change in a pipe r_i is a function of the mean density $\rho_{\mathrm{m}}(p_{\mathrm{m}})$, the geometrical volume V_{geo} and the mass of the pipe at the beginning of each hour:

$$\Delta m_{\mathrm{r},i} = \Delta m \cdot \left(\frac{\rho_{\mathrm{m},i}(p_{\mathrm{m},i}) \cdot V_{\mathrm{geo},i} - m_{\mathrm{r},i}}{\sum_j \rho_{\mathrm{m},j}(p_{\mathrm{m},j}) \cdot V_{\mathrm{geo},j} - m_{\mathrm{r},j}} \right) \qquad (5)$$

The mean pressure p_{m} is determined using the integral mean value according to Mischner [5] in a numerically stable form:

$$p_{\mathrm{m}} = \frac{2}{3} \cdot \left(p_2 + \frac{p_1 \cdot p_1}{p_1 + p_2} \right) \qquad (6)$$

The mean density $\rho_{\mathrm{m}}(p_{\mathrm{m}})$ is determined using a simplified virial equation taking the real gas behaviour into account. To calculate the virial coefficients B_i and the molar mass M_i, the SGERG equation is used once for all entry nodes [6]. The material properties are propagated through the gas grid weighted by volume:

$$\rho_{\mathrm{m}} = -\frac{1}{2 \cdot B_i} - \sqrt{\left(\frac{1}{2 \cdot B_i} \right)^2 + \frac{p_{\mathrm{m}} \cdot M_i}{R_{\mathrm{m}} \cdot T \cdot B_i}} \quad (7)$$

The mass flows $\dot{m}_{\mathrm{r},i}$ are calculated with respect to of the mass changes $\Delta m_{\mathrm{r},i}$ (Eq. (5)) of the individual pipes by solving a linear equation system, and are used to determine the flow velocities u_i and the associated pressure losses Δp_i:

$$u_i = \frac{\dot{m}_{\mathrm{r},i}}{\rho_{\mathrm{m},i}(p_{\mathrm{m},i}) \cdot A_i} \qquad (8)$$

The pressure losses Δp_i are computed according to Darcy-Weisbach [5,7] with the use of Zanke's approach [8,9] for determining the friction factor of the pipe λ_{m}. The index 1 indicates the entry into the pipe:

$$\Delta p_i = p_{1,i} \cdot \left(1 - \sqrt{1 - \lambda_{m,i} \cdot \frac{L_i}{D_i} \cdot \frac{\rho_{1,i}}{p_{1,i}} \cdot u_{1,i}{}^2} \right) \quad (9)$$

Zanke's approach provides a consistent method for describing the friction factor of the pipe over the entire laminar and turbulent range, which is valid both for hydraulically smooth and for hydraulically rough pipes.

$$\lambda = \lambda_{\mathrm{turb}} \cdot \alpha + \lambda_{\mathrm{lam}} \cdot (1 - \alpha) \qquad (10)$$

Where:

$$\lambda_{\mathrm{turb}} = \left[-2 \cdot \lg \left(2.7 \cdot \frac{(\lg(\mathrm{Re}))^{1.2}}{\mathrm{Re}} + \frac{k}{3.71 \cdot D} \right) \right]^{-2} \quad (11)$$

$$\lambda_{\mathrm{lam}} = \frac{64}{\mathrm{Re}} \qquad (12)$$

$$\alpha = \exp\big(-\exp(-(0.0025 \cdot \mathrm{Re} - 6.75)) \big) \qquad (13)$$

Evaluations of different regional distribution grids have shown that 90 % of the flow velocities vary from 0.1 m/s to 2.0 m/s. Therefore nearly 10 % of the state of flow is laminar i.e. the Reynolds number Re is less than 2300:

$$\mathrm{Re} = \frac{u \cdot \rho \cdot D}{\eta} \qquad (14)$$

The calculated pressure losses Δp_i are used to determine the node pressures p_k in the gas grid. For a given pressure distribution, the mean grid pressure is iterated until the mass $m_{\mathrm{r},i}$ of all pipes for a given mass change $\Delta m_{\mathrm{r},i}$ equals the mass obtained by the product of mean density $\rho_{\mathrm{m}}(p_{\mathrm{m}})$ and geometrical volume V_{geo}.

An iterative process is necessary because pressure distribution and mass distribution determine one another reciprocally. After each iteration the flow velocities, mass flows and pressures are used to compute the new distribution of material data such as H_{s}, ρ_{n} and B_i in the gas grid.

4 VALIDATION OF THE KERNEL

The SmartSim kernel which has been validated with data from the 2011 field trial carried out in a distribution grid operated by Avacon [10]. Calibrated measurements were carried out at different exit points with a mobile process gas chromatograph (PGC). The grid topology as well as the locations of the mobile PGC are shown in Figure 2. A comparison was also carried out with established reference software [11] for transmission grids.

Table 1 shows a comparison between the measured CVs $H_{\mathrm{s,meas}}$ and the CVs calculated with SmartSim $H_{\mathrm{s,new}}$ on a monthly basis. Maximum deviations of ±0.1 % are observed. In addition the deviations of SmartSim from the CVs $H_{\mathrm{s,Ref}}$ of the reference software are shown. With deviations of less than ±0.01 %, differences between SmartSim using the new kernel and the reference software are not significant.

The SmartSim kernel was validated further by evaluating the relative CV difference for every hour and node with the reference software ac-

cording to Eq. (15). A comparison of pressures, flow velocities and volume flows was also performed. Because the CV distribution in gas grids depends on the these parameters, only results for CV deviations are shown. The evaluation comprised 671,140 hourly values and was done in an extended time period from 01.12.2010 to 01.10.2011.

$$\Delta H_s = \frac{H_{s,\text{new}} - H_{s,\text{Ref}}}{H_{s,\text{Ref}}} \qquad (15)$$

Figure 3 shows the deviation of the SmartSim kernel from the reference as a histogram with relative frequency density. The mean deviation of $\bar{H}_s$ = 0.01 % shows that no significant systematic deviations occur. The standard deviation is around σ = 0.35 %. All in all the resulting form of the histogram is much narrower than a normal distribution with the same standard deviation, indicating minimal deviations between the SmartSim kernel and the software for transmission grids.

Table 1 Comparison of measured and calculated calorific values during the field trial.

Month	SmartSim	Measurement		Reference	
	$H_{s,\text{new}}$	$H_{s,\text{meas}}$	$\Delta H_{s,\text{meas}}$	$H_{s,\text{Ref}}$	$\Delta H_{s,\text{Ref}}$
	kWh/m^3	kWh/m^3	%	kWh/m^3	%
12.2010	11.368	11.369	0.01	11.368	0.00
01.2011	11.334	11.338	0.04	11.334	0.00
02.2011	11.338	11.337	-0.01	11.338	0.00
03.2011	11.275	11.277	0.02	11.274	-0.01
04.2011	11.273	11.283	0.09	11.273	0.00
05.2011	11.353	11.353	0.00	11.352	-0.01
06.2011	11.355	11.354	-0.01	11.355	0.00
07.2011	11.308	11.307	-0.01	11.309	0.01
08.2011	11.211	11.213	0.02	11.211	0.00

The computation time needed for the hydraulic simulation of one month for the Lüchow grid is approx. 0.4 s for the SmartSim kernel. The benchmark was carried out on an Intel Core i5-3320m with 2.6 GHz running with Windows 8.1. The computing time for the evaluation of the regional distribution grid which we studied is thus far shorter than with established systems.
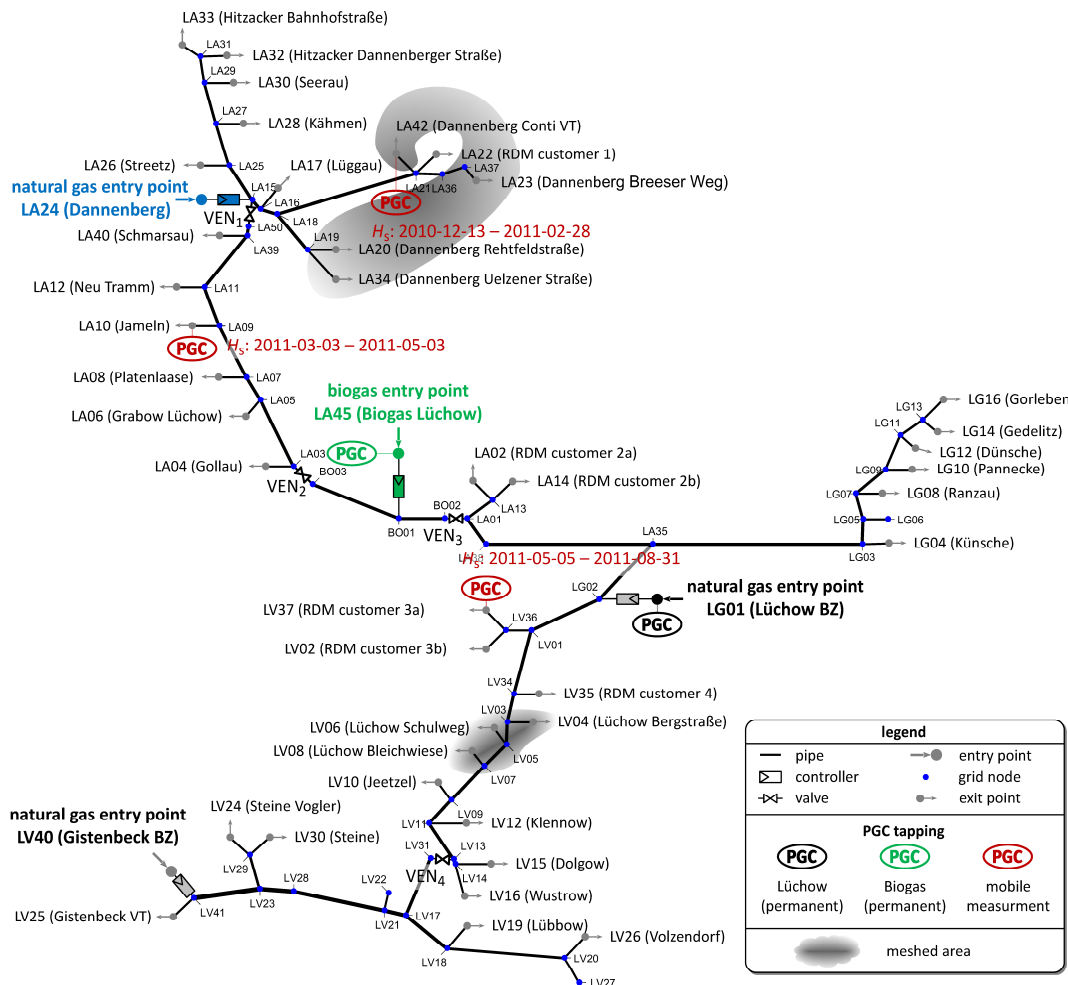

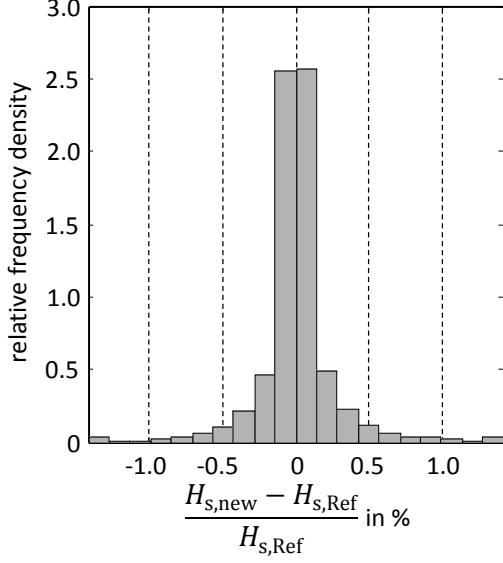Figure 2 Topology of the evaluated Lüchow distribution grid.

Figure 3 Deviation of the new kernel and reference software.

5 Uncertainty Calculation by Monte Carlo Simulation

As part of this study, a comprehensive uncertainty calculation for CV tracking was carried out for the first time based on the "Guide to the Expression of Uncertainty in Measurement" (GUM) [12]. A Monte Carlo Simulation according to GUM S2 [13] is well suited for this task due to the very complex nature of distribution grids and their often limited measuring infrastructure. The simulation determines the relation between the uncertainties of the input variables and the resulting uncertainty of the billing CV empirically. All input variables are varied place in parallel and randomly distributed in so-called scenarios. The scenario with unchanged input variables is referred to as reference scenario (Ref) in the following. Determining the uncertainty for a 95 % confidence interval requires a minimum of 1537 scenarios, so the number of scenarios is set at N_{MC} = 1600 below. The volume-weighted billing CVs $\overline{H}_s$ of scenario j at node i in month T are each compared with the billing CV of the reference scenario $\overline{H}_s^{Ref}$ (see Eq. (16)):

$$\delta\overline{H}_{s,j,i,T} = \frac{\overline{H}_{s,j,i,T} - \overline{H}_{s,i,T}^{Ref}}{\overline{H}_{s,i,T}^{Ref}} \qquad (16)$$

The standard uncertainty $u(\delta\overline{H}_{s,i,T})$ is obtained with Eq. (17) and is converted with a coverage factor k = 2 to form the expanded measurement uncertainty $U(\delta\overline{H}_{s,i,T})$. For the arithmetical examination of the method, the standard un-

certainties u listed in Table 2 were assumed for the input variables shown in Figure 1.

$$u(\delta\overline{H}_{s,i,T})$$

$$= \sqrt{\frac{1}{N_{MC} - 1} \cdot \sum_{j=1}^{N_{MC}} \left(\delta\overline{H}_{s,j,i,T} - E(\delta\overline{H}_{s,i,T})\right)^2} \qquad (17)$$

Two different uncertainty distributions are used: The normal (n) distribution indicating the standard uncertainty and a continuous uniform (rectangular, r) distribution in the value range $[E - 3u \ldots E + 3u]$, where E represents the mean value. For evaluation purposes all normally distributed standard uncertainties are converted to rectangular distributions to rule out e.g. physically impossible negative SLP energy offtakes due to major errors outside the 3-u interval. Finite interval limits combined with a constant probability density of the rectangular distribution increase the resulting standard uncertainty u_{res} by the factor $\sqrt{3}$ compared with the standard uncertainty u of the standard deviation. On completion of the Monte Carlo Simulation, the expanded measurement uncertainty $U(\delta\overline{H}_{s,i,T})$ is plotted in a bar chart for each node and month, see Figure 4. The variation of the input variables was derived using a pseudo random generator. To ensure the repeatability of results, the random generator was initialized with a fixed number before the first MC scenario.

The expanded measurement uncertainty $U(\delta\overline{H}_{s,i,T})$ varies largely between the different exit nodes and hence essentially on the flow situation within the grid. It should be noted that the uncertainties shown in Table 2 represent very conservative estimates and that this also affects the resulting uncertainties. The entry CVs of natural gas und biomethane were also set at an artificial difference of 7.4 % to simulate unconditioned biomethane. 95 % of all expanded uncertainties $U(\delta\overline{H}_{s,i,T})$ are less than or equal to 0.43 %. All expanded uncertainties remain within the maximum limit of 2 % [2]. The results of the field trial also indicate far smaller actual deviations than the calculated uncertainties (see Table 1). An outlying maximum uncertainty of $U(\delta\overline{H}_{s,i,T}) \leq 0.90$ % occurred at a volume-measured exit point in April. The gas offtake in this month was not continuous and was less than 100 m³. This high uncertainty in April can be disregarded compared with the total offtake quantity of 4.5 million m³ per annum.

Table 2 Standard uncertainties of input variables for the Monte Carlo Simulation (MCS).

| Variable	standard uncertainty			MCS
	type	u	u_{res}	distribution
pipe roughness	rectangular	[0.001 ... 0.1]	52.0 %	[20 % ... 200 %]
pipe length	normal	5 %	8.7 %	[85 % ... 115 %]
pipe diameter	normal	2 %	3.5 %	[94 % ... 106 %]
SLP-Energy 1 (systematic, all nodes)	normal	10 %	17.3 %	[70 % ... 130 %]
SLP-Energy 2 (systematic, individual nodes)	normal	10 %	17.3 %	[70 % ... 130 %]
SLP-Energy 3 (hourly value, all nodes)	normal	10 %	17.3 %	[70 % ... 130 %]
measured offtake	normal	1 %	1.7 %	[97 % ... 103 %]
entry volume	normal	1 %	1.7 %	[97 % ... 103 %]
entry pressure	normal	2 %	3.5 %	[94 % ... 106 %]
gas temperature	rectangular	[3°C ... 13 C]	1.0 %	[98.2 % ... 101.8 %]
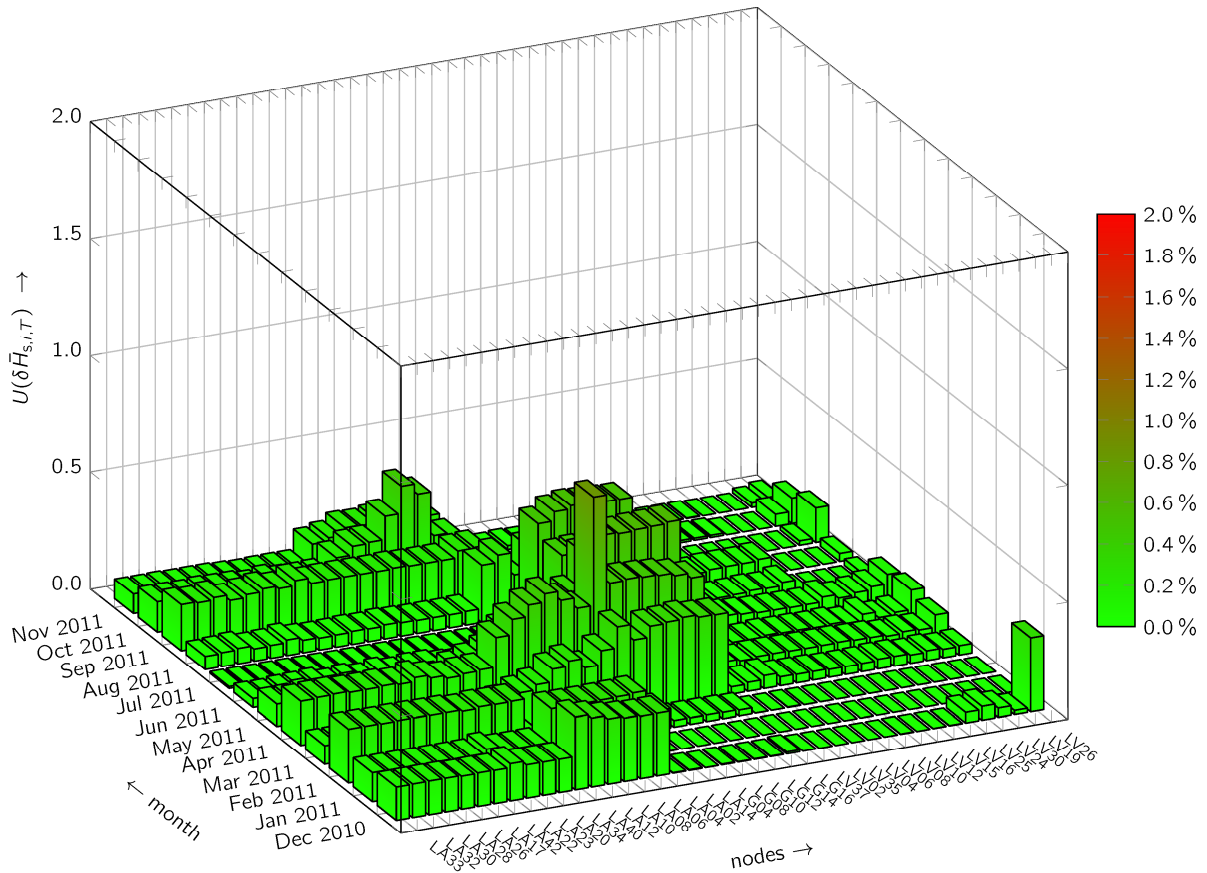
Figure 4 Uncertainty of the simulated gas flow $U(\delta\bar{H}_{s,i,T})$ expanded by k = 2 of the mean relative CV deviation $\delta\bar{H}_{s,i,T}$ per node i and month T as per N_{MC} = 1600 Monte Carlo scenarios.

6 CONCLUSIONS AND OUTLOOK

This article presents a newly developed kernel for the simulation of gas distribution grids. This kernel offers a high level of accuracy and extremely short computation times. Complex grids can be calculated very efficiently by integrating the new kernel into the SmartSim software developed by E.ON Technologies for CV tracking. The kernel is being validated using measurements with a mobile process gas chromatograph and by comparing it with established simulation software. The concordances found for flow velocities, volume flow rates and calorific values are excellent. In addition, for the first time an uncertainty evaluation for the calculated calorific values was carried out using a Monte Carlo Simulation according to the "Guide to the Expression of Uncertainty in Measurement". The results are presented here for illustration by reference to a regional distribution grid operated by Avacon.

The expanded uncertainties remained below the maximum limit of 2 % despite a conservative estimate of the input uncertainties. Current investigations focus on the use of the new SmartSim kernel for transmission grids.

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