

SIMULATION OF CRITICAL NOZZLE FLOW CONSIDERING REAL GAS EFFECTS

*P. Schley¹, E. von Lavante², D. Zeitz², M. Jaeschke¹, H. Dietrich³
and B. Nath³*

¹ Elster Produktion GmbH, Steinernstrasse 19-21, D-55252 Mainz-Kastel, Germany

² Institute of Turbomachinery, University of Essen, D-45127 Essen, Germany

³ Ruhrgas AG, Halterner Strasse 125, D-46284 Dorsten, Germany

Abstract: Critical nozzle flow is predicted for high pressure natural gas by way of numerical simulation. The CFD-program used was developed for simulating two-dimensional and axially symmetric, viscous flow. The thermodynamic properties significantly affecting nozzle flow of high pressure natural gas were computed using the AGA8-DC92 equation of state. To verify the present theoretical results, mass flow measurements of natural gas were made using the Pigsar high-pressure test rig. A comparison between theoretical and experimental results is presented for one test case.

Keywords: Critical Flow Factor, Critical Nozzle, Discharge Coefficient, Natural Gas, Numerical Simulation, Real Gas

1 INTRODUCTION

Critical nozzles are widely used as a reference standard in gas flow measurements. Apart from a high reproducibility of measurements, main benefits include easy handling and short adjustment times. The mass flow of the gas as described in ISO 9300 [1] involves the critical flow factor, C^* , which depends on the thermodynamic properties of the gas, and the discharge coefficient, C_D , determined mainly by nozzle geometry. For pure substances or air, there are relatively simple computation methods ([1],[2]) for computing the C^* and C_D , providing very accurate results. In the case of natural gas, the mass flow is not only a function of pressure and temperature, but also of the composition, making a theoretical description far more difficult. Particularly under high pressure (e.g. 2 - 5 MPa), a precise description of the thermodynamic properties of the gas as well as viscous effects are essential for accurate mass flow determination.

In this paper, theoretical flow prediction is performed by way of numerical simulation using a field computational method. The program, called „ACHIEVE“, based on the solution of the two-dimensional or axisymmetric Navier Stokes equation [3], has been developed to simulate compressible, viscous, unsteady nozzle flows. Numerous program simulations were carried out for air at atmospheric pressure and verified by measurements. In this work, ACHIEVE was to be used for high pressures natural gases. In order to determine the relevant thermodynamic properties of natural gases (including density, entropy, enthalpy, speed of sound) as accurately as possible, the AGA8-DC92 equation of state [4] was implemented in ACHIEVE.

Numerical simulation using ACHIEVE represents suitable means to predict critical nozzle flow. The program is to be used for the design/dimensioning of critical nozzles and specification of calibration methods.

2 DETERMINATION OF THERMAL AND CALORIC PROPERTIES OF NATURAL GAS

With the AGA8-DC92 equation of state [4], compression factor and density of natural gases can be determined over a wide range of pressures and temperatures with high accuracy. The equation designated AGA8 in the following requires as input a detailed 21-component gas analysis.

To apply the AGA8 equation for computing caloric properties, an additional equation is required to formulate caloric behaviour in the ideal gas state as a function of temperature, e.g. ideal gas heat capacity c_p^0 . A previous paper [5] developed equations formulating ideal gas heat capacity c_p^0 as a function of temperature for the 21 components also reflected by the AGA8 equation.

The above procedure is the most accurate computation method for thermal and caloric natural gas properties available. The GERG project [6] (Groupe Européen de Recherches Gazières) conducted comprehensive tests to check the various equations of state against measured values and came to the same positive conclusion regarding the present method.

3 DETERMINATION OF CRITICAL FLOW FACTOR C^* FOR REAL GASES

The critical flow factor C^* describes the effects of thermodynamic property of one-dimensional isentropic nozzle flow between the inlet and the throat of the nozzle.

$$C^* = \rho^* \cdot a^* \frac{\sqrt{R_s \cdot T_0}}{\rho_0} \quad (1)$$

In order to determine the critical flow factor C^* as a function of the stagnation conditions, following ideal conditions must be met:

- (i) Nozzle flow must be isentropic (entropie $s = \text{const.}$, $s_* = s_0$).
- (ii) Nozzle is considered adiabatic, meaning total enthalpy between the inlet and the throat of the nozzle is constant ($h_*^t = h_0^t$).
- (iii) Flow velocity across nozzle throat is equal to local speed of sound ($u_* = a_*$).

With these conditions, the critical flow condition (P^* , T^*) and thus the critical flow factor C^* are clearly specified and can be calculated using the iterative procedure presented in Fig. 1. However, a caloric equation of state is required to determine enthalpy, entropy, speed of sound and density as a function of pressure, temperature and gas composition. In this paper, we use the AGA8 equation [4], as presented in Section 2.

The input parameters p_0 and T_0 are used in the first step to calculate enthalpy h_0 and entropy s_0 . A preliminary critical flow condition is determined using a starting value for p^* . Subsequently, the values for T_* , h_* , a_* and u_* can be computed using the AGA8 equation. The truncation criterion $|\Delta| < 10^{-5}$ m/s ensures that condition (iii) requiring flow velocity to be equal to local speed of sound is satisfied with acceptable accuracy. If the truncation criteria is not met, which is usually the case during the first iteration, a new value is determined for pressure p^* . In order to determine a new pressure value, the actual p^* value is increased by an infinitesimal amount ∂p to obtain p'^* . Then equations (2) to (6) are solved again to calculate the difference $\Delta' = a'^* - u'^*$. In this way, we can determine the sensitivity ($\partial\Delta/\partial p$) of the difference Δ with respect to p^* , which is then used to specify a new pressure value. The procedure is repeated until the truncation criterion is satisfied, normally after two to three iteration steps. The values determined for a_* , T_* and p_* are then used to determine density ρ^* and subsequently the critical flow factor C^* using equation (1).

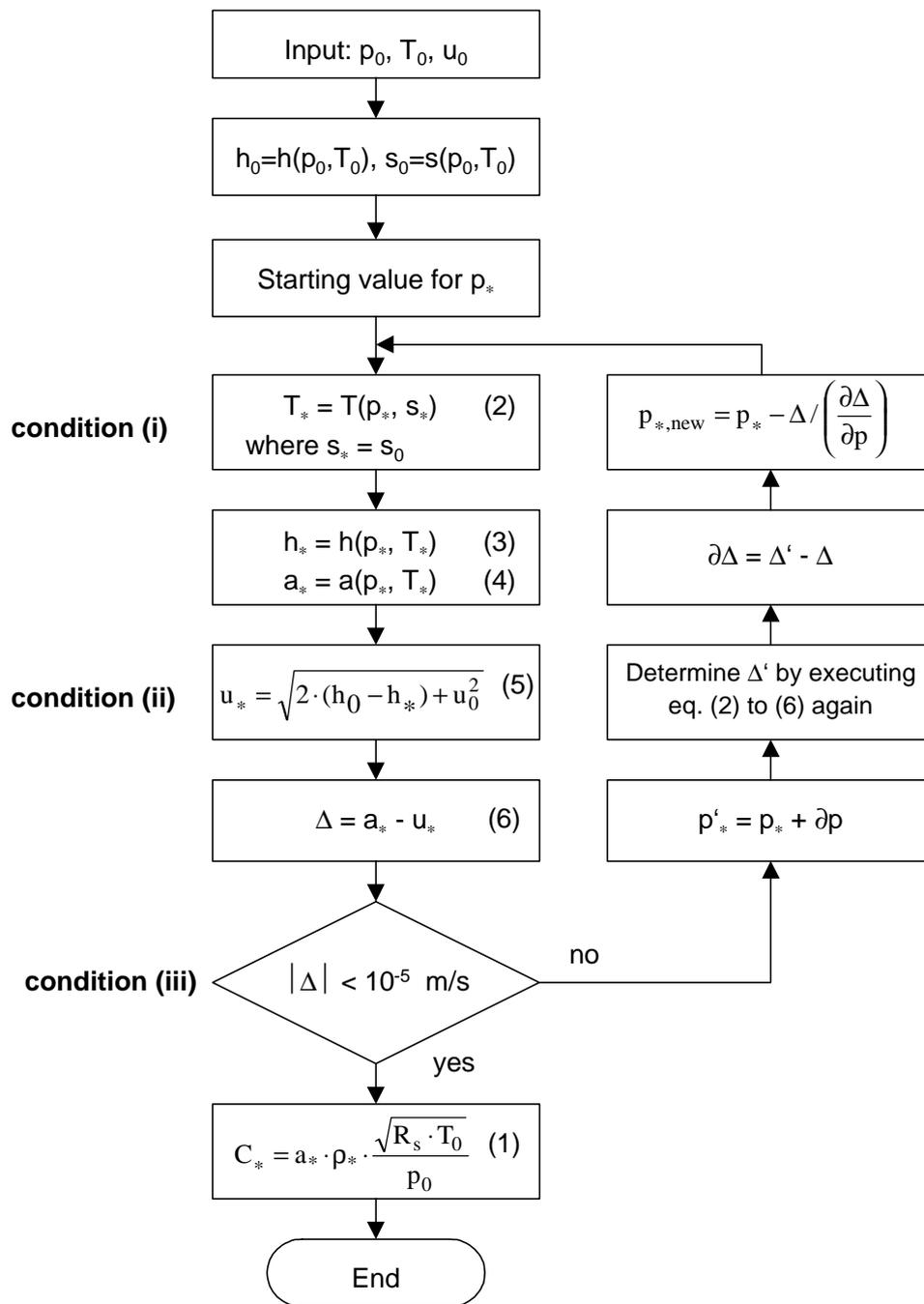


Fig. 1: Iterative procedure to determine the critical flow factor C^* using the AGA8 equation [4].

4 REAL GAS EFFECTS

In order to describe the influence of real gas effects on critical nozzle flow, the numerical procedure described in Section 3 was employed for various gases. Methane, a low-calorific natural gas with a high nitrogen mole fraction ($x_{N_2} = 11.7$ mol%) and a high calorific natural gas with a high ethane mole fraction ($x_{C_2H_6} = 8.5$ mol%) were examined. The gases selected are extreme examples with respect to thermodynamic behaviour considering the natural gases shipped by Ruhrgas.

The stagnation pressure p_0 was varied over the range of 0 to 5 MPa and the local speed of sound a_* and the flow factor C_* were computed. Fig. 2 shows the results. The respective intersection points with the ordinate for $p = 0$ represent the values describing the ideal gas state.

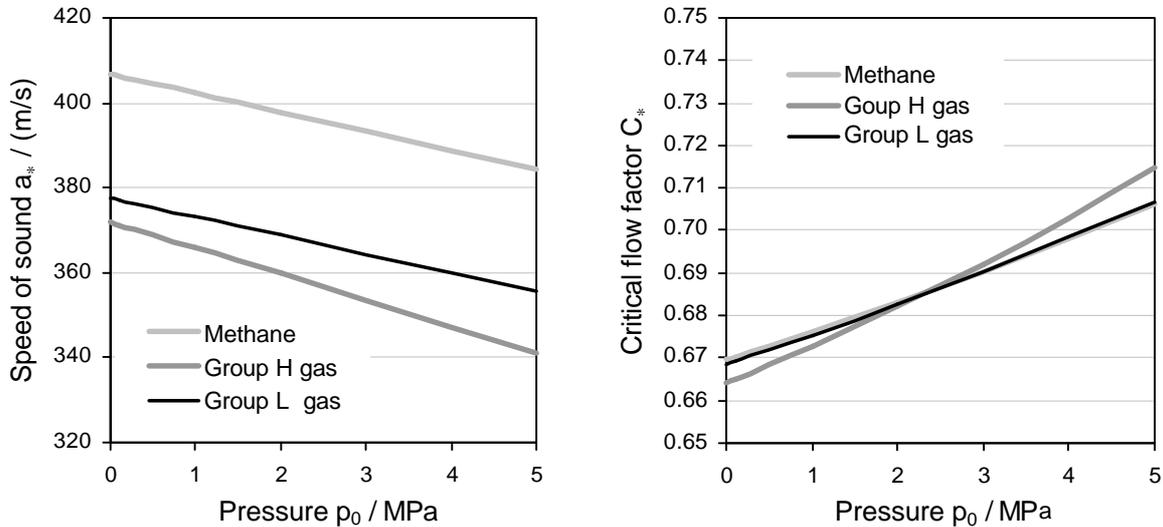


Fig. 2: Speed of sound a_* and critical flow factor C_* as a function of pressure p_0 for methane, group L gas and group H gas ($T_0 = 293.15$ K).

Speed of sound is strongly dependent on gas type. The values obtained for pure methane are 8 to 10 % higher than for the natural gas group H and 7 % higher than for the natural gas group L. Real gas effects at 5 MPa cause speed of sound to be reduced by 5.5 % for methane and NAM gas and 8 % for Ekofisk gas.

The critical flow factor increases continuously as stagnation pressure p_0 increases. In the case of the group H gas, the difference compared with the ideal gas state is as high as 1.5 % at $p_0 = 1$ MPa; at $p_0 = 5$ MPa the difference is 9.2 %. Real gas effects are somewhat lower for the other gases.

5 NUMERICAL SIMULATION OF A TWO-DIMENSIONAL NOZZLE FLOW USING ACHIEVE

The numerical method employed in the present flow simulations is part of a flow simulation system developed at the Institute of Turbomachinery at the University of Essen, called "ACHIEVE". It consists of an upwind solver of the Navier-Stokes equations, using the finite volume discretization. The governing equations to be solved in the present simulations are the two-dimensional or axisymmetric compressible Navier-Stokes equations. The full Navier-Stokes equations are given in detail by, for example, Steger [7] or von Lavante and Groenner [3].

Due to the complexity of the predicted flow, a simple numerical scheme with central spatial differences and artificial dissipation added explicitly was not suited for the present simulations. Therefore, the well known and proven Roe's Scheme [8] was employed. The numerical scheme is based on Roe's Flux Difference Splitting in finite volume form, as developed by von Lavante et. al. [9]. The method has been proven to be accurate and effective in the simulation of viscous flows with wide range of Mach numbers [3].

The governing equations were integrated in time by solving their semidiscrete form by means of either modified Runge-Kutta (R-K) time stepping or implicit symmetric Gauß-Seidel (SGS) relaxation method. In the present work, the two stage version of the R-K procedure was utilized. The corresponding Runge-Kutta coefficients α_i were optimized by von Lavante et. al. [10] for maximum multigrid performance (damping of high frequencies). That optimization was done, however, using a

linear hyperbolic model equations. In realistic applications, these coefficients worked fine for the inviscid Euler equations as well as for most viscous cases. The simple two stage R-K procedure was as efficient as the more frequently used four stage scheme, but required only one optimized coefficient, $\alpha_1 = 0.42$.

The simulations were carried out on structured grids. The mesh points were arranged according to an algebraic distribution and clustered at the solid walls to ensure enough gridpoints in the boundary layers. The domain was divided into several blocks in order to make the formulation of the boundary conditions and handling complex geometries easier. Furthermore, the Multiblock-structure was necessary to compute the flow on parallel computers. More details about the present numerical method are given in accompanying paper [11].

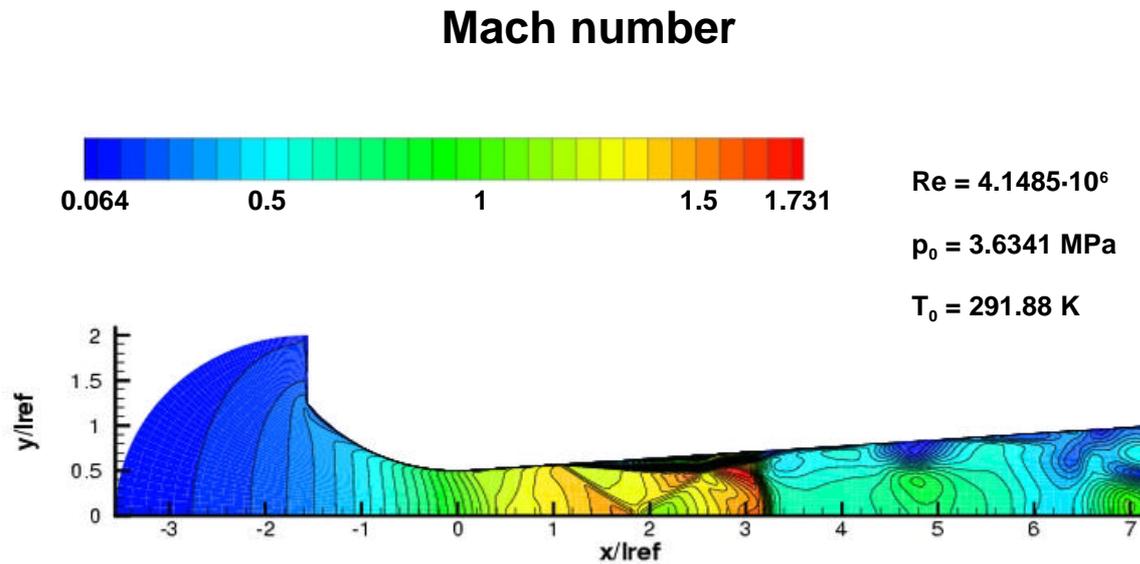


Fig. 3: Mach number plot over nozzle geometry for a given time instant.

In Fig. 3, a computed flow field for the Mach number at one given time instant is displayed. The picture reveals that the flow is steady upstream of the throat as well as downstream up to the first oblique shock. An oblique shock is produced due to the developing boundary layer at the nozzle wall ($x/l_{ref} \approx 1.1$); the shock then assumes reflection like structure at the symmetric line ($x/l_{ref} \approx 1.9$). The shock interacts for a second time with the separated boundary layer farther downstream ($x/l_{ref} \approx 2.6$). The following almost normal shock ($x/l_{ref} \approx 3.2$) produces a significant pressure increase that causes a massive periodic boundary layer separation coupled with vortex shedding. After the shock, the flow is unsteady and the separation area is convected to the outlet of the nozzle.

All these unsteady effects are downstream the supersonic flow region and therefore do not influence the flow in the throat. The simulation shown in Fig. 3 was also used for discharge coefficient determination in the following section.

6 COMPARISON OF SIMULATION RESULTS WITH MEASURED VALUES

Critical nozzle measurements were made using natural gas in the Ruhrgas Pigsar high-pressure test rig in Dorsten, Germany. The natural gas considered is a low-calorific gas with approx. 10 mol% of nitrogen. Reference [12] gives an overview of the test set-up and a description of the measured results. This paper uses one measurement as an example to check measured massflow against theoretical values obtained from numerical simulation and other computation methods.

The measurement considered here was performed with a 9.94 mm dia. nozzle. The stagnation conditions were $p_0 = 3.6341$ MPa and $T_0 = 291.88$ K. The results are presented in Table 1:

Table 1: Calculated mass flows vs. experimental value ($Q_{m,exp} = 0.5404$ kg/s).

calculation method ¹	A	B	C	D
critical flow factor C^*	0.6672	0.6938	0.6961	0.6961
discharge coefficient C_D	1	0.9929	0.9929	0.9970
mass flow $Q_m /$ (kg/s)	0.5203	0.5372	0.5390	0.5412
deviation from experiment $\Delta Q_m / \%$	-3.71	-0.59	-0.26	0.15

¹ The following methods were used for calculating C^* and C_D :

- A:** C^* in accordance with ISO 9300 [1] for ideal gas ($K = 1.3$), $C_D = 1$.
- B:** C^* and C_D in accordance with ISO 9300.
- C:** C^* using AGA8 equation [4] (see Section 3), C_D to ISO 9300 [1].
- D:** C^* using AGA8 equation [4] (see Section 3), C_D with ACHIEVE (this paper).

In accordance with ISO Standard 9300, the mass flows shown in Table 1 are determined from:

$$Q_m = C^* \cdot C_D \cdot A^* \frac{p_0}{\sqrt{R_s \cdot T_0}} \quad (7)$$

Various calculation methods are considered for determination of the critical flow factor C^* and discharge coefficient C_D . Case A proceeds from the simplifying assumption that ideal gas behaviour applies ($Z = 1$, $K_0 = 1.3 = \text{const.}$) and that flow is one-dimensional and does not involve friction ($C_D = 1$). The other methods are based on real gas nozzle flow. In case B, both C^* and C_D are calculated in accordance with ISO Standard 9300. The C^* calculation method of ISO 9300 agrees with the paper by Johnson [13] and is based on the older equation of state by Benedict Webb Rubin [14]. Case C calculates the critical flow factor C^* on the basis of the AGA8 equation [4] using the method presented in Section 3; the C_D coefficient is calculated in accordance with ISO Standard 9300. Case D is also based on C^* calculated using the AGA8 equation; C_D is obtained from numerical simulation under ACHIEVE.

Table 1 shows the best agreement between calculated and experimental value for case D ($\Delta Q_m = 0.15\%$). The mass flows determined for cases B and C were calculated with the same C_D coefficient, but with different critical flow factors C^* . The values deviate from measured mass flow by -0.59% and -0.26% , respectively. This indicates that the calculation method presented in Section 3 is more accurate than the method in accordance with ISO Standard 9300 or Reference [13]. This was also confirmed by further measurements. As expected, the case A calculation which is to illustrate once again real gas effects on mass flow determination involves the greatest deviation ($\Delta Q_m = -3.71\%$).

REFERENCES

- [1] ISO 9300 Measurement of Gas Flow by Means of Critical Flow Venturi Nozzles (1990).
- [2] D. G. Stewart, J. T. R. Watson, and A. M. Vaidya: Improved Critical Flow Factors and Representative Equations for Four Calibration Gases. *Flow Measurement and Instrumentation* 10 (1999) No. 1, 27-34
- [3] E. von Lavante, and J. Groenner: Semiimplicit Schemes for Solving the Navier-Stokes Equations. *9th GAMM Conference*, Lausanne, Notes on Numerical Fluid Mechanics, Vieweg, 1992.
- [4] K. E. Starling, and J. L. Savidge: Compressibility Factors of Natural Gas and Other Related Hydrocarbon Gases. *American Gas Association Transmission Measurements Committee Report No. 8*, Second Edition, Arlington 1992 and Errata No. 1, June 1993.
- [5] M. Jaeschke and P. Schley: Ideal-Gas Thermodynamic Properties for Natural Gas Applications. *Int. J. Thermophys.* Vol. 16 (1995) No. 6, p. 1381/1392.
- [6] R. Klimeck, R. Span, R. Kleinrahm, W. Wagner: Fundamental Equation for Calorific Properties. Report by Ruhr-Universität Bochum, Chair of Thermodynamics (1996).
- [7] J. L. Steger: Implicit, Finite-Difference Simulation of Flow about Arbitrary Geometries. *AIAA Journal*, Vol. 16 (1978) No. 7.
- [8] P. L. Roe: Approximate Riemann Solvers, Parameter Vectors and Difference Schemes. *J. Comp. Phys.*, Vol. 43 (1981) 357-372.
- [9] E. von Lavante, A. El-Milligui and H. A. Warda: Simulation of Unsteady Flows Using Personal Computers. *The 3rd Int. Congress on Fluid Mechanics*, Cairo (1990).
- [10] E. von Lavante, A. El-Milligui, F. E. Canizzaro and H. A. Warda: Simple Explicit Upwind Schemes for Solving Compressible Flows. *Proceedings of the 8th GAMM Conference on Numerical Methods in Fluid Mechanics*, Delft (1990).
- [11] E. von Lavante, M. Ishibashi and G. Wendt: Investigation of Flowfields in Small Sonic Venturi-Nozzles. *Proceedings of the International Conference "FLOMEKO 2000"* (Salvador, 4-8. June 2000), Salvador, Brasil.
- [12] H. Dietrich, B. Nath, P. Schley, M. Jaeschke, E. von Lavante and G. Wendt: Flow Meter Calibration with Sonic Nozzles in High Pressure Natural Gas. *Proceedings of the International Conference "FLOMEKO 2000"* (Salvador, 4-8. June 2000), Salvador, Brasil.
- [13] R. C. Johnson: Calculation of the Flow of Natural Gas Through Critical Flow Nozzles. *Journal of Basic Engineering* 92 (1970) No. 3, 580-589.
- [14] M. Benedict, G. B. Webb, L. Rubin: An Empirical Equation for Thermodynamic Properties of Light Hydrocarbons and their Mixtures: Constants for twelve Hydrocarbons. *Chem. Eng. Prog.* 47, 8 (1951) 419-422.

Authors

- 1 Ruhrgas AG, Energy Measurement, Instrumentation & Control, Simulation, Halterner. Str. 125, 46284 Dorsten, Germany. E-mail: Peter.Schley@ruhrgas.com, Manfred.Jaeschke@ruhrgas.com
- 2 Institute of Turbomachinery, University of Essen, 45127 Essen, Germany. E-mail: Erni@tigger.turbo.uni-essen.de, Fox@tigger.turbo.uni-essen.de
- 3 Elster Produktion GmbH, R&D Department, Steinernstrasse19-21, 55252 Mainz-Kastel, Germany. E-mail: dietrich@elster.com, nath@elster.com