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## MODELLING OF VISCOUS TURBULENT FLOW IN FLOW PARTS OF TURBINES FOR ORC PLANTS WITH TAKING INTO ACCOUNT THE REAL PROPERTIES OF THE WORKING FLUID MDM ON THE BASIS OF THE MODIFIED BENEDICT-WEBB-RUBIN EQUATION OF STATE

The paper describes a modified form of the Benedict-Webb-Rubin thermal equation of state with 32 members received on the basis of its thermodynamic functions. The developed method of interpolation-analytical approximation of the modified Benedict-Webb-Rubin equation of state accounts for the real properties of working medium in 3D calculations. Constants of the equation of state are selected by on the basis of available thermodynamic property tables. On the one hand, it allows for sufficient accuracy, and on the other - does not require a significant increase in computational cost. The proposed method is validated using a sample working fluid – MDM (silica oil), which is used in ORC cycles of low-power cogeneration plants. It is shown that the mBWR32 equation with the obtained constants provides a good accuracy in the whole range of variation of thermodynamic values in the gaseous state and on the saturation line.

**Keywords:** Benedict-Webb-Rubin equation of state, interpolation-analytical approximation, the free Helmholtz energy.

### Introduction

In modeling of spatial gas dynamic processes on the basis of numerical integration of the Reynolds-averaged Navier-Stokes equations, it is necessary to establish the connection between the thermodynamic quantities in the form of a state equation. Currently, the most common equations of state used in the three-dimensional computations are equations of perfect gas, Tammann and Van der Waals equations. Unfortunately, in many cases, these equations do not provide the required accuracy of the results. A remedy could be the equation of Benedict-Webb-Rubin, which is one of the most universal and reliable equations of state. A direct use of this equation in three-dimensional calculations is currently not possible, because in that case the computing time is increased by 1.5 - 2 orders of magnitude.

The paper presents a modified form of the Benedict-Webb-Rubin thermal equation of state with 32 members (mBWR32). A method for the determination of constants of the modified Benedict-Webb-Rubin equation is proposed on the basis of the available tables of thermodynamic quantities. The presented interpolation-analytical method of approximation of complex thermodynamic functions is, on the one side, sufficient to ensure a meaningful accuracy, and on the other side, does not require a substantial increase in the computational cost. It is also shown that the quadruple precision of calculations (32 significant digits in floating point operations) is needed for the determination of the con-

stants as well as for the calculation of thermodynamic parameters.

The proposed method is validated using a sample working fluid – MDM, which is used in ORC cycles of low-power cogeneration plants. It is shown that the mBWR32 equation with the obtained constants provides a good accuracy in the whole range of variation of thermodynamic values in the gaseous state and on the saturation line.

### Modified benedict-webb-rubin equation of state. Basic thermodynamic functions

The thermally modified Benedict-Webb-Rubin equation of state of with 32 members [1] has the form:

$$\begin{aligned}
 P = \rho RT + \rho^2 \left[ G(1)T + G(2)T^{1/2} + G(3) + \frac{G(4)}{T} + \frac{G(5)}{T^2} \right] \\
 + \rho^3 \left[ G(6)T + G(7) + \frac{G(8)}{T} + \frac{G(9)}{T^2} \right] + \\
 + \rho^4 \left[ G(10)T + G(11) + \frac{G(12)}{T} \right] + \rho^5 [G(13)] + \\
 + \rho^6 \left[ \frac{G(14)}{T} + \frac{G(15)}{T^2} \right] + \rho^7 \left[ \frac{G(16)}{T} \right] + \\
 + \rho^8 \left[ \frac{G(17)}{T} + \frac{G(18)}{T^2} \right] + \rho^9 \left[ \frac{G(19)}{T^2} \right] + \\
 + \rho^3 \left[ \frac{G(20)}{T^2} + \frac{G(21)}{T^3} \right] \exp(\gamma\rho^2) +
 \end{aligned}$$

$$\begin{aligned}
 & +\rho^5 \left[ \frac{G(22)}{T^2} + \frac{G(23)}{T^4} \right] \exp(\gamma\rho^2) + \\
 & +\rho^7 \left[ \frac{G(24)}{T^2} + \frac{G(25)}{T^3} \right] \exp(\gamma\rho^2) + \\
 & +\rho^9 \left[ \frac{G(26)}{T^2} + \frac{G(27)}{T^4} \right] \exp(\gamma\rho^2) + \\
 & +\rho^{11} \left[ \frac{G(28)}{T^2} + \frac{G(29)}{T^3} \right] \exp(\gamma\rho^2) + \\
 & +\rho^{13} \left[ \frac{G(30)}{T^2} + \frac{G(31)}{T^3} + \frac{G(32)}{T^4} \right] \exp(\gamma\rho^2). \quad (1)
 \end{aligned}$$

For the simulation of spatial viscous flows it is necessary to know thermodynamic dependencies for the following values:  $u$ ;  $h=u+P/\rho$ ;  $C_v$ ;  $C_p$ ;  $S$ ;  $a$ . To determine these dependencies, differential equations of thermodynamics [2], equation (1) and a dependence for the Helmholtz free energy  $f$  are used. The Helmholtz free energy can be introduced into equation (1) using the expression:

$$P = \rho^2 \left( \frac{\partial f}{\partial \rho} \right)_T. \quad (2)$$

Equation (2) allows us to express the Helmholtz free energy  $f$  in the form of an arbitrary polynomial with respect to  $T$ . In this paper, the expression for the Helmholtz free energy taken in the form:

$$f = f_i + f_v, \quad (3)$$

where

$$\begin{aligned}
 f_i &= RT \ln(\rho) + \\
 & + \rho \left[ G(1)T + G(2)\sqrt{T} + G(3) + \frac{G(4)}{T} + \frac{G(5)}{T^2} \right] + \\
 & + \frac{\rho^2}{2} \left[ G(6)T + G(7) + \frac{G(8)}{T} + \frac{G(9)}{T^2} \right] + \\
 & + \frac{\rho^3}{3} \left[ G(10)T + G(11) + \frac{G(12)}{T} \right] + \frac{\rho^4}{4} G(13) + \\
 & + \frac{\rho^5}{5} \left[ \frac{G(14)}{T} + \frac{G(15)}{T^2} \right] + \frac{\rho^6}{6} \frac{G(16)}{T} + \\
 & + \frac{\rho^7}{7} \left[ \frac{G(17)}{T} + \frac{G(18)}{T^2} \right] + \frac{\rho^8}{8} \frac{G(19)}{T^2} + \\
 & + \frac{G(33)}{T} + G(34)T + G(35)T^2 + G(36)T \ln(T) + G(37); \\
 f_v &= I_1 \left[ \frac{G(20)}{T^2} + \frac{G(21)}{T^3} \right] + I_2 \left[ \frac{G(22)}{T^2} + \frac{G(23)}{T^4} \right] + \\
 & + I_3 \left[ \frac{G(24)}{T^2} + \frac{G(25)}{T^3} \right] + I_4 \left[ \frac{G(26)}{T^2} + \frac{G(27)}{T^4} \right] + \\
 & + I_5 \left[ \frac{G(28)}{T^2} + \frac{G(29)}{T^3} \right] + I_6 \left[ \frac{G(30)}{T^2} + \frac{G(31)}{T^3} + \frac{G(32)}{T^4} \right];
 \end{aligned}$$

$$I_1 = \int \rho \exp(\gamma\rho^2) d\rho = \frac{1}{2\gamma} \exp(\gamma\rho^2);$$

$$I_2 = \int \rho^3 \exp(\gamma\rho^2) d\rho = \frac{\gamma\rho^2 - 1}{2\gamma^2} \exp(\gamma\rho^2);$$

$$\begin{aligned}
 I_3 &= \int \rho^5 \exp(\gamma\rho^2) d\rho = \\
 &= \frac{\gamma^2\rho^4 - 2\gamma\rho^2 + 2}{2\gamma^3} \exp(\gamma\rho^2);
 \end{aligned}$$

$$\begin{aligned}
 I_4 &= \int \rho^7 \exp(\gamma\rho^2) d\rho = \\
 &= \frac{\gamma^3\rho^6 - 3\gamma^2\rho^4 + 6\gamma\rho^2 - 6}{2\gamma^4} \exp(\gamma\rho^2);
 \end{aligned}$$

$$\begin{aligned}
 I_5 &= \int \rho^9 \exp(\gamma\rho^2) d\rho = \\
 &= \frac{\gamma^4\rho^8 - 4\gamma^3\rho^6 + 12\gamma^2\rho^4 - 24\gamma\rho^2 + 24}{2\gamma^5} \exp(\gamma\rho^2);
 \end{aligned}$$

$$\begin{aligned}
 I_6 &= \int \rho^{11} \exp(\gamma\rho^2) d\rho = \\
 &= \frac{\left( \gamma^5\rho^{10} - 5\gamma^4\rho^8 + 20\gamma^3\rho^6 - \right.}{\left. -60\gamma^2\rho^4 + 120\gamma\rho^2 - 120 \right) \exp(\gamma\rho^2)}{2\gamma^6}.
 \end{aligned}$$

An additional polynomial comprising five members is supplemented to equation (3), which leads to an increase in the number of constants  $G$  from 32 to 37. This polynomial yields zero value to equation (1). In view of (1) and (3) the required thermodynamic functions take the form as below:

The internal energy:

$$u = f - T \left( \frac{\partial f}{\partial T} \right)_\rho, \quad (4)$$

where  $\left( \frac{\partial f}{\partial T} \right)_\rho = \left( \frac{\partial f_i}{\partial T} \right)_\rho + \left( \frac{\partial f_v}{\partial T} \right)_\rho$ ;

$$\begin{aligned}
 \left( \frac{\partial f_i}{\partial T} \right)_\rho &= R \ln(\rho) + \\
 & + \rho \left[ G(1) + \frac{1}{2} \frac{G(2)}{\sqrt{T}} - \frac{G(4)}{T^2} - 2 \frac{G(5)}{T^3} \right] + \\
 & + \frac{\rho^2}{2} \left[ G(6) - \frac{G(8)}{T^2} - 2 \frac{G(9)}{T^3} \right] + \\
 & + \frac{\rho^3}{3} \left[ G(10) - \frac{G(12)}{T^2} \right] + \frac{\rho^5}{5} \left[ -\frac{G(14)}{T^2} - 2 \frac{G(15)}{T^3} \right] - \\
 & - \frac{\rho^6}{6} \frac{G(16)}{T^2} + \frac{\rho^7}{7} \left[ -\frac{G(17)}{T^2} - 2 \frac{G(18)}{T^3} \right] - \\
 & - \frac{\rho^8}{4} \frac{G(19)}{T^3} - \frac{G(33)}{T^2} + G(34) + \\
 & + 2G(35)T + G(36) + G(36) \ln(T);
 \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial f_v}{\partial T}\right)_\rho &= I_1 \left[ -2 \frac{G(20)}{T^3} - 3 \frac{G(21)}{T^4} \right] + \\ &+ I_2 \left[ -2 \frac{G(22)}{T^3} - 4 \frac{G(23)}{T^5} \right] + \\ &+ I_3 \left[ -2 \frac{G(24)}{T^3} - 3 \frac{G(25)}{T^4} \right] + \\ &+ I_4 \left[ -2 \frac{G(26)}{T^3} - 4 \frac{G(27)}{T^5} \right] + \\ &+ I_5 \left[ -2 \frac{G(28)}{T^3} - 3 \frac{G(29)}{T^4} \right] + \\ &+ I_6 \left[ -2 \frac{G(30)}{T^3} - 3 \frac{G(31)}{T^4} - 4 \frac{G(32)}{T^5} \right]. \end{aligned}$$

*Isochoric heat capacity:*

$$\begin{aligned} c_v &= \left(\frac{\partial u}{\partial T}\right)_\rho = \left(\frac{\partial f}{\partial T}\right)_\rho - \left(\frac{\partial f}{\partial T}\right)_\rho - \\ &- T \left(\frac{\partial^2 f}{\partial T^2}\right)_\rho = -T \left(\frac{\partial^2 f}{\partial T^2}\right)_\rho, \end{aligned}$$

where  $\left(\frac{\partial^2 f}{\partial T^2}\right)_\rho = \left(\frac{\partial^2 f_i}{\partial T^2}\right)_\rho + \left(\frac{\partial^2 f_v}{\partial T^2}\right)_\rho$ ;

$$\begin{aligned} \left(\frac{\partial^2 f_i}{\partial T^2}\right)_\rho &= \rho \left[ -\frac{1}{4} \frac{G(2)}{T^2} + 2 \frac{G(4)}{T^3} + 6 \frac{G(5)}{T^4} \right] + \\ &+ \frac{\rho^2}{2} \left[ 2 \frac{G(8)}{T^3} + 6 \frac{G(9)}{T^4} \right] + \frac{2}{3} \rho^3 \frac{G(12)}{T^3} + \\ &+ \frac{\rho^5}{5} \left[ 2 \frac{G(14)}{T^3} + 6 \frac{G(15)}{T^4} \right] + \frac{\rho^6}{3} \frac{G(16)}{T^3} + \\ &+ \frac{\rho^7}{7} \left[ 2 \frac{G(17)}{T^3} + 6 \frac{G(18)}{T^4} \right] + \frac{3}{4} \rho^8 \frac{G(19)}{T^4} + \\ &+ 2 \frac{G(33)}{T^3} + 2G(35) + \frac{G(36)}{T}; \\ \left(\frac{\partial^2 f_v}{\partial T^2}\right)_\rho &= I_1 \left[ 6 \frac{G(20)}{T^4} + 12 \frac{G(21)}{T^5} \right] + \\ &+ I_2 \left[ 6 \frac{G(22)}{T^4} + 20 \frac{G(23)}{T^6} \right] + I_3 \left[ 6 \frac{G(24)}{T^4} + 12 \frac{G(25)}{T^5} \right] + \\ &+ I_4 \left[ 6 \frac{G(26)}{T^4} + 20 \frac{G(27)}{T^6} \right] + I_5 \left[ 6 \frac{G(28)}{T^4} + 12 \frac{G(29)}{T^5} \right] + \\ &+ I_6 \left[ 6 \frac{G(30)}{T^4} + 12 \frac{G(31)}{T^5} + 20 \frac{G(32)}{T^6} \right] \end{aligned}$$

*Isobaric heat capacity:*

$$\begin{aligned} c_p &= \left(\frac{\partial h}{\partial T}\right)_p = \left[\frac{\partial}{\partial T} \left(u + \frac{P}{\rho}\right)\right]_p = \left(\frac{\partial u}{\partial T}\right)_p - \frac{P}{\rho^2} \left(\frac{\partial \rho}{\partial T}\right)_p = \\ &= \left(\frac{\partial f}{\partial T}\right)_p - \left(\frac{\partial f}{\partial T}\right)_\rho - T \left[\frac{\partial \left(\frac{\partial f}{\partial T}\right)_\rho}{\partial T}\right]_p - \frac{P}{\rho^2} \left(\frac{\partial \rho}{\partial T}\right)_p = \\ &= -T \left[\frac{\partial \left(\frac{\partial f}{\partial T}\right)_\rho}{\partial T}\right]_p = -T \left[\left(\frac{\partial^2 f}{\partial T^2}\right)_\rho + \frac{A}{\rho^2} \left(\frac{\partial \rho}{\partial T}\right)_p\right] = \\ &= -T \left[\left(\frac{\partial^2 f}{\partial T^2}\right)_\rho - \frac{A^2}{\rho^2 B}\right] = c_v + \frac{A^2 T}{\rho^2 B}, \end{aligned} \tag{6}$$

where

$$\begin{aligned} A &= \rho R + \rho^2 \left[ G(1) + \frac{1}{2} \frac{G(2)}{\sqrt{T}} - \frac{G(4)}{T^2} - 2 \frac{G(5)}{T^3} \right] + \\ &+ \rho^3 \left[ G(6) - \frac{G(8)}{T^2} - 2 \frac{G(9)}{T^3} \right] + \rho^4 \left[ G(10) - \frac{G(12)}{T^2} \right] + \\ &+ \rho^6 \left[ -\frac{G(14)}{T^2} - 2 \frac{G(15)}{T^3} \right] - \rho^7 \left[ \frac{G(16)}{T^2} \right] + \\ &+ \rho^8 \left[ -\frac{G(17)}{T^2} - 2 \frac{G(18)}{T^3} \right] - 2\rho^9 \left[ \frac{G(19)}{T^3} \right] + \\ &+ \rho^3 \left[ -2 \frac{G(20)}{T^3} - 3 \frac{G(21)}{T^4} \right] \exp(\gamma \rho^2) + \\ &+ \rho^5 \left[ -2 \frac{G(22)}{T^3} - 4 \frac{G(23)}{T^5} \right] \exp(\gamma \rho^2) + \\ &+ \rho^7 \left[ -2 \frac{G(24)}{T^3} - 3 \frac{G(25)}{T^4} \right] \exp(\gamma \rho^2) + \\ &+ \rho^9 \left[ -2 \frac{G(26)}{T^3} - 4 \frac{G(27)}{T^5} \right] \exp(\gamma \rho^2) + \\ &+ \rho^{11} \left[ -2 \frac{G(28)}{T^3} - 3 \frac{G(29)}{T^4} \right] \exp(\gamma \rho^2) + \\ &+ \rho^{13} \left[ -2 \frac{G(30)}{T^3} - 3 \frac{G(31)}{T^4} - 4 \frac{G(32)}{T^5} \right] \exp(\gamma \rho^2); \\ B &= RT + 2\rho \left[ G(1)T + G(2)\sqrt{T} + G(3) + \frac{G(4)}{T} + \frac{G(5)}{T^2} \right] + \\ &+ 3\rho^2 \left[ G(6)T + G(7) + \frac{G(8)}{T} + \frac{G(9)}{T^2} \right] + \end{aligned}$$

$$\begin{aligned}
 &+4\rho^3 \left[ G(10)T + G(11) + \frac{G(12)}{T} \right] + \\
 &+5\rho^4 [G(13)] + 6\rho^5 \left[ \frac{G(14)}{T} + \frac{G(15)}{T^2} \right] + \\
 &+7\rho^6 \left[ \frac{G(16)}{T} \right] + 8\rho^7 \left[ \frac{G(17)}{T} + \frac{G(18)}{T^2} \right] + \\
 &+9\rho^8 \left[ \frac{G(19)}{T} \right] + (3\rho^2 + 2\gamma\rho^4) \left[ \frac{G(20)}{T^2} + \frac{G(21)}{T^3} \right] * \\
 &* \exp(\gamma\rho^2) + (5\rho^4 + 2\gamma\rho^6) * \left[ \frac{G(22)}{T^2} + \frac{G(23)}{T^4} \right] \exp(\gamma\rho^2) + \\
 &+ (7\rho^6 + 2\gamma\rho^8) \left[ \frac{G(24)}{T^2} + \frac{G(25)}{T^3} \right] \exp(\gamma\rho^2) + \\
 &+ (9\rho^8 + 2\gamma\rho^{10}) \left[ \frac{G(26)}{T^2} + \frac{G(27)}{T^4} \right] \exp(\gamma\rho^2) + \\
 &+ (11\rho^{10} + 2\gamma\rho^{12}) \left[ \frac{G(28)}{T^2} + \frac{G(29)}{T^3} \right] \exp(\gamma\rho^2) \\
 &+ (13\rho^{12} + 2\gamma\rho^{14}) \left[ \frac{G(30)}{T^2} + \frac{G(31)}{T^3} + \frac{G(32)}{T^4} \right] \exp(\gamma\rho^2).
 \end{aligned}$$

Entropy:

$$S = - \left( \frac{\partial f}{\partial T} \right)_\rho. \quad (7)$$

Sonic speed:

$$\begin{aligned}
 a^2 &= \left( \frac{\partial P}{\partial \rho} \right)_S = \frac{T \left( \frac{\partial P}{\partial T} \right)_\rho + c_V \left( \frac{\partial T}{\partial v} \right)_P}{\rho^2 c_V \left( \frac{\partial T}{\partial P} \right)_\rho} = \\
 &= \frac{T \left( \frac{\partial P}{\partial T} \right)_\rho + c_V \rho^2 \left( \frac{\partial T}{\partial \rho} \right)_P}{\rho^2 c_V \left( \frac{\partial T}{\partial P} \right)_\rho} = B + \frac{TA^2}{c_V \rho^2}.
 \end{aligned} \quad (8)$$

### Method of interpolation-analytical approximation of the thermodynamic functions

For the first time, this method was applied in the three-dimensional calculation to account for the thermodynamic properties of water and steam based on the equation of state IAPWS-95 [3, 4]. Under this approach, the required thermodynamic functions were determined by the dependencies:

$$\begin{aligned}
 T &= \frac{p}{\rho R z_t(\rho, p)}; \quad \rho = \frac{p}{h} z_\rho(h, p); \\
 u &= \frac{p z_u(\rho, p)}{\rho z_t(\rho, p)}; \quad p = \rho \cdot u \cdot z_p(\rho, u);
 \end{aligned}$$

$$\begin{aligned}
 a &= \sqrt{\frac{p z_a(\rho, p)}{\rho z_t(\rho, p)}}; \quad h = \frac{p}{\rho} \left( 1 + \frac{z_u(\rho, p)}{z_t(\rho, p)} \right); \\
 C_V &= R \cdot z_{C_V}(\rho, p); \quad S = R \cdot z_S(\rho, p); \\
 u_p &= \frac{z_u(\rho, p)}{\rho \cdot z_t(\rho, p)}; \quad u_\rho = - \frac{p z_u(\rho, p)}{\rho z_t(\rho, p)}; \quad S_p = \frac{C_V}{p}; \\
 S_\rho &= - \frac{C_p}{\rho}; \quad T_p = \frac{1}{\rho R \cdot z_t(\rho, p)}; \\
 T_\rho &= - \frac{p}{\rho^2 R \cdot z_t(\rho, p)}, \quad (9)
 \end{aligned}$$

where  $z_t(\rho, p)$ ,  $z_\rho(h, p)$ ,  $z_u(\rho, p)$ ,  $z_p(\rho, u)$ ,  $z_{C_V}(\rho, p)$ ,  $z_{C_p}(\rho, p)$ ,  $z_S(\rho, p)$  – the dimensionless compressibility coefficients for the corresponding thermodynamic functions determined by interpolation from a pre-calculated arrays of the base points. To reduce the dimension of the array without a loss of accuracy, independent variables – the pressure and density - are considered in a logarithmic scale.

Values of the dimensionless compressibility coefficients are defined in the base points as:

$$\begin{aligned}
 z_t &= \frac{p}{\rho RT}; \quad z_u = \frac{u}{RT}; \quad z_\rho = \frac{h p}{p}; \\
 z_p &= \frac{p}{\rho \cdot u}; \quad z_a = \frac{a^2}{RT}; \quad z_{C_V} = \frac{C_V}{R}; \\
 z_{C_p} &= \frac{C_p}{R}; \quad z_S = \frac{S}{R}, \quad (10)
 \end{aligned}$$

where corresponding values  $p$ ,  $\rho$ ,  $T$ ,  $u$ ,  $h$ ,  $a$ ,  $C_p$ ,  $C_V$  and  $S$  are calculated using the thermodynamic relations (1, 4-8).

### Determination of constants for the equation of state

Usually, constants for equations of state are determined based on the experimental data. In the literature, one can find information about values of the constants of simple equations of state for various types of working medium [2]. Open information about values of constants for the modified Benedict-Webb-Rubin equation of state with 32 members is available only for a narrow range of working medium [1]. However, there are various software packages that allow us to calculate the array of fields of thermodynamic functions for any working medium. Theoretically, these arrays can be directly used in the determination of the coefficients (10). Using the existing software, it is usually possible to obtain arrays of a few hundred points only. However, to maintain the high accuracy of three-dimensional gas dynamics calculations, the dimension of arrays should typically be as high as a few million. Therefore, in the described method the obtained arrays of thermodynamic function values are used to determine the necessary constants of Benedict-Webb-Rubin equation of state,

and then new arrays of the required dimension are calculated with the help of equations (1, 4-8).

The gas constant  $R$  is determined as a ratio of the universal gas constant to the molecular weight of the considered working medium. The remaining constants  $\gamma$ ,  $G$  are determined using the least squares method [5, 6] to assure the smallest square deviation of the dimensionless unknown function from the array base point values:

$$\sum_{i=1}^n \left( \frac{f_i - y_i}{y_i} \right)^2 \rightarrow \min, \quad (11)$$

where  $f_i$  – the required thermodynamic function of the modified Benedict-Webb-Rubin equation of state at point  $i$  of the array;  $y_i$  – value of the thermodynamic function at point  $i$ ;  $n$  – dimension of the base points array. The problem (11) can be solved in the following way. If  $\gamma$  is assumed as known and constant, then the condition (11) can be replaced by the condition (12):

$$\sum_{i=1}^n \sum_{j=1}^{37} \left( \frac{f_i - y_i}{y_i^2} \frac{\partial f_i}{\partial G_j} \right) = 0, \quad (12)$$

where  $j$  is the number of constants  $G$ . The expression (12) is a system of 37 linear equations with respect to 37 unknowns  $G$  for the thermodynamic functions: the pressure, Helmholtz free energy, entropy and the partial derivative of pressure with density at constant temperature. The linear system of equations (12) is solved by the Gauss method with dominant diagonal terms [5, 6]. The accuracy of calculations is set at quadruple precision with 32 characters. Such a large mantissa is needed to maintain the required high accuracy. The global search for the problem (11) is carried out by varying  $\gamma$  in the range:

$$-100\rho_*^2 \leq \gamma \leq 100\rho_*^2, \quad (13)$$

where  $\rho_*$  is the value of the density at the critical point. Constants are found for the simultaneous fulfillment of condition (11) for the following thermodynamic functions: pressure, the Helmholtz free energy, entropy, and the partial derivative of pressure with respect to density at constant temperature.

To validate the functionality of the method, sample detailed numerical investigations were carried out for the expansion line of four last stages (stages 4-7) of a 100 kW ORC cogeneration turbine operating on MDM as a working medium [7, 8]. The meridional section of the turbine flow part is presented in Figure 1, whereas stator and rotor profiles of the investigated stages 4-7 are illustrated in Figure 2. The calculations were performed with the following boundary conditions:

- inlet parameters upstream of stage 4:
  - pressure: 2.76 bar;
  - temperature: 530.4 K;
- outlet parameters:
  - pressure: 0.17 bar;

- rotational speed: 9000 rev/min.

3D numerical investigations of flow were made with the help of the software complex *IPMFlow*, which is the development of the software systems *FlowER* and *FlowER-U*. It implements the following elements of the mathematical model: the unsteady Reynolds-averaged Navier-Stokes equations, SST Menter differential two-equation turbulence model, implicit quasi-monotone high-order ENO-scheme [9, 10].

A base point array of values of thermodynamic functions was obtained with the help of the program REFPROP [11] in 735 points within the entire range of pressure and temperature available for this medium in REFPROP. The following values of constants were obtained:

$R = 0.3515168000E+02$ ;  
 $\gamma = -0.262270170807420121513573739971D-04$   
 $G(01) = 0.302207868111278740060411592544D+00$   
 $G(02) = -0.495233944170545289062576542307D+01$   
 $G(03) = -0.225501201197491314642998011829D+03$   
 $G(04) = 0.107906234213802120996678810443D+06$   
 $G(05) = -0.372657132543797518687633762851D+08$   
 $G(06) = -0.627320725108084212417049028312D-03$   
 $G(07) = 0.215743936748432144179678929724D+01$   
 $G(08) = -0.192205460461420765746900736543D+04$   
 $G(09) = 0.517361137204233382712063500157D+06$   
 $G(10) = 0.766264823125748039322791551715D-06$   
 $G(11) = -0.434353699956369187362735134447D-02$   
 $G(12) = 0.161657815774704243989178292974D+01$   
 $G(13) = 0.288814234808349750753865171475D-05$   
 $G(14) = 0.227250568997175780038146727298D-04$   
 $G(15) = -0.652886158820518451942746541068D-02$   
 $G(16) = -0.456739733049471206918455720386D-07$   
 $G(17) = 0.231242587293920118661113372857D-10$   
 $G(18) = 0.186380264921967994590840358405D-07$   
 $G(19) = -0.126528342901003631469807144831D-10$   
 $G(20) = 0.347527618252179836075855868907D+06$   
 $G(21) = -0.160950582611693360862236427413D+09$   
 $G(22) = 0.693289101786031245959518372491D+01$   
 $G(23) = -0.953438468030805490987102326088D+06$   
 $G(24) = 0.297824147414970198157551618564D-03$   
 $G(25) = -0.230534235531245981576803850333D+00$   
 $G(26) = -0.213236230412490644485878013528D-08$   
 $G(27) = 0.167631613366536556924666638381D-02$   
 $G(28) = 0.904911503767510905693979818203D-13$   
 $G(29) = -0.704815505181047779157572048773D-10$   
 $G(30) = -0.501394975086843725544491118562D-18$   
 $G(31) = 0.454671117815342747169810491557D-15$   
 $G(32) = -0.539871248063102930246035212608D-13$   
 $G(33) = 0.117126880134545422586004289266D+09$   
 $G(34) = 0.140470196549871558017639577219D+05$   
 $G(35) = -0.469999084243383589981287193248D+00$   
 $G(36) = -0.193705173670445390344105907111D+04$   
 $G(37) = -0.116961966600901591984328215895D+07.$

(14)

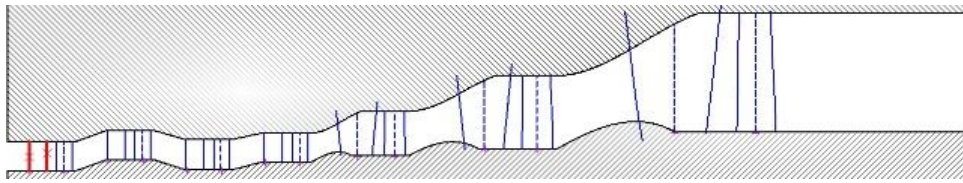


Figure 1. The meridional section of the flow part

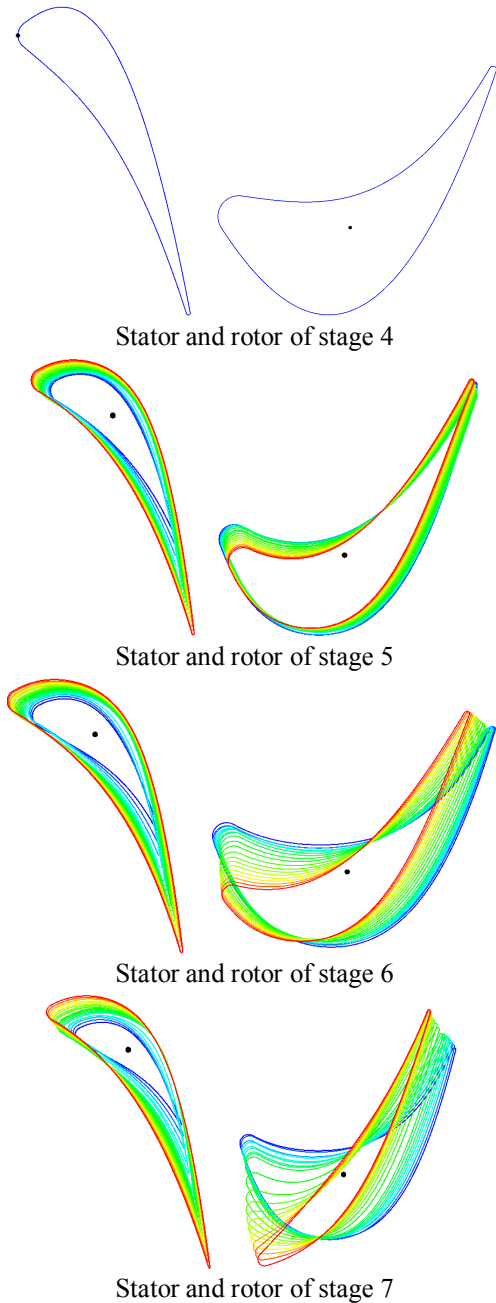


Figure 2. Hub-to-tip profile sections for stage 4-7

With the above constants (14), the mean square deviation of values of thermodynamic functions (1, 4-8) from the array base point values is equal to 0.02%, whereas the maximum square deviation does not exceed 0.17%.

Figure 3 shows sample visualisation of flow patterns in the investigated turbine stages obtained from 3D calculations with the modified Benedict-Webb-Rubin equation of state. The pictures of velocity vectors exhibit regular flow patterns and a relatively high flow efficiency.

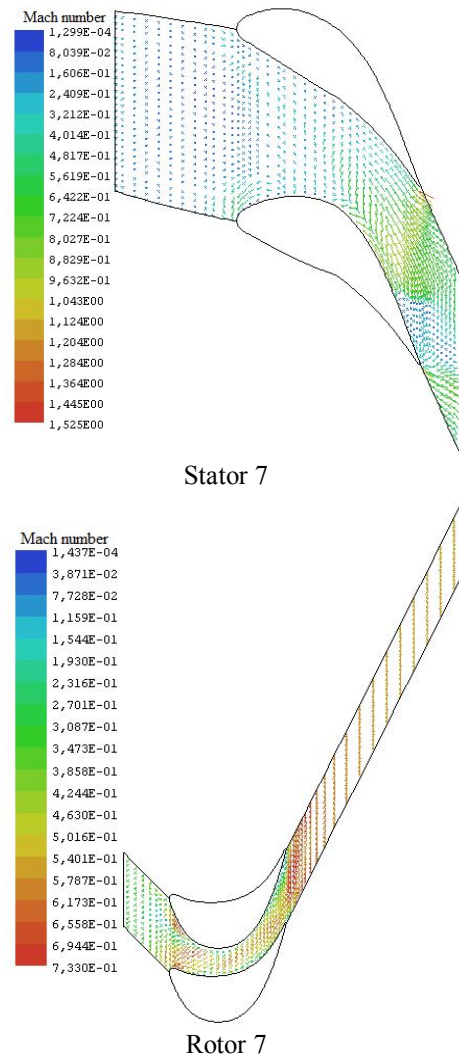


Figure 3. Velocity vectors at the last stage

The calculations using the methodology of interpolation-analytical approximation of the modified Benedict-Webb-Rubin equation of state with 32 members are compared with those of the Tammann equation of state:

$$p + p_0 = R \rho T . \quad (15)$$

Constants for the Tammann equation were evaluated from static inlet parameters and isentropic outlet parameters of the working medium:

$$\begin{aligned} \gamma &= 1.019; \\ c_p &= 1689.8 \text{ J/(kg}\cdot\text{K)}; \\ R &= 31.64 \text{ J/(kg}\cdot\text{K)}; \\ P_0 &= -1613.07 \text{ Pa.} \end{aligned} \quad (16)$$

Tables 1 and 2 show the comparison of results obtained from the two considered state equations. The comparison of flow parameters in the axial gaps downstream of subsequent stages is given in Table 1, whereas integral characteristics of the stages and stage group are gathered in Table 2.

The calculations using the modified Benedict-Webb-Rubin equation of state exhibit slightly larger drops of pressure, temperature and enthalpy in subsequent stages and predict higher flow efficiency in the calculated turbine stages. In the presented case, the differences between the results shown in Tables 1-2 are not that significant.

Table 1  
Comparative characteristics of steam parameters  
in the axial gaps

Stage №	Equation of state	P out, bar	T, K	$\Delta h$ , J/kg
4	Tammann	1.53	525.3	8431
	mBWR32	1.54	524.6	8597
5	Tammann	0.8	519.7	9609
	mBWR32	0.79	518.7	9943
6	Tammann	0.4	513.7	10126
	mBWR32	0.39	512.8	10650
7	Tammann	0.17	505.9	13208
	mBWR32	0.17	505.7	13310

Table 2  
Comparative characteristics of integral characteristics

Stage №	Equation of state	$\eta$ , %	N, kW
4	Tammann	83.94	12.8
	mBWR32	87.12	13.2
5	Tammann	87.33	15.75
	mBWR32	86.92	16.1
6	Tammann	87.97	17.35
	mBWR32	87.36	18.1
7	Tammann	90.94	21.8
	mBWR32	90.75	21.55
4-7	Tammann	87.99	67.7
	mBWR32	88.32	69.1

This is due to the fact that in this flow part, the absolute values of pressure, temperature and enthalpy drops are not that high and, most important, because MDM belongs to the class of dry fluids. The differences are expected to be much higher for wet medium with phase transitions within the expansion range. More investigations will be carried for both dry and wet me-

dium, including water vapour, and they will soon be validated by experimental data.

## Conclusion

The method of interpolation-analytical approximation of the modified Benedict-Webb-Rubin equation of state was developed to account for real properties of working medium in three-dimensional flow calculations. Constants of the modified Benedict-Webb-Rubin equation of state with 32 members were determined on the basis of the available arrays of thermodynamic functions, values. The method allows us on the one hand to provide a sufficient accuracy, and on the other hand does not require a significant increase in computational cost. Test calculations of the last 4 stages of a 100 kW ORC turbine with MDM as a working medium are presented. It is shown that the proposed method of determination of the state equation constants yields the standard deviation of 0.02% and the maximum deviation of 0.17% from the array values. Differences in evaluation of flow parameters using the modified Benedict-Webb-Rubin equation of state and Tammann equation in the axial gaps downstream of the subsequent stages are also described. These results will soon be validated by experimental data.

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### **МОДЕЛИРОВАНИЕ ПРОСТРАНСТВЕННОГО ВЯЗКОГО ТЕЧЕНИЯ В ПРОТОЧНЫХ ЧАСТЯХ ТУРБИН ДЛЯ ОРС УСТАНОВОК С УЧЕТОМ РЕАЛЬНЫХ СВОЙСТВ РАБОЧЕГО ТЕЛА MDM НА ОСНОВЕ МОДИФИЦИРОВАННОГО УРАВНЕНИЯ СОСТОЯНИЯ БЕНЕДИКТА-ВЕББА-РУБИНА**

*А. Русанов, П. Лампарт, Р. Русанов*

Приведен вид модифицированного термического уравнения состояния Бенедикта-Вебба-Рубина с 32 членами, а также полученных на его основе термодинамических функций. Разработан метод интерполяционно-аналитической аппроксимации модифицированного уравнения состояния Бенедикта-Вебба-Рубина для учета реальных свойств рабочих тел в трехмерных расчетах. Константы уравнения состояния выбираются на основе имеющихся термодинамических таблиц свойств. С одной стороны, это позволяет обеспечить достаточную точность, а с другой – не требует существенного увеличения вычислительных затрат. Проверка предложенного метода проводилась для рабочего тела – MDM (силикатное масло), которое используется в ОРС циклах когенерационных установок малой мощности. Показано, что модифицированное уравнение состояния Бенедикта-Вебба-Рубина с определенными константами обеспечивает хорошую точность во всем диапазоне изменения термодинамических величин в газообразном состоянии и вблизи линии насыщения.

**Ключевые слова:** уравнение состояния Бенедикта-Вебба-Рубина, интерполяционно-аналитическая аппроксимация, свободная энергия Гельмгольца.

### **МОДЕЛЮВАННЯ ПРОСТОРОВОЇ В'ЯЗКОЇ ТЕЧІЇ В ПРОТОЧНИХ ЧАСТИНАХ ТУРБІН ДЛЯ ОРС УСТАНОВОК З УРАХУВАННЯМ РЕАЛЬНИХ ВЛАСТИВОСТЕЙ РОБОЧОГО ТІЛА MDM НА ОСНОВІ МОДИФІКОВАНОГО РІВНЯННЯ СТАНУ БЕНЕДИКТА-ВЕББА-РУБІНА**

*А. Русанов, П. Лампарт, Р. Русанов*

Наведено вид модифікованого термічного рівняння стану Бенедикта-Вебба-Рубіна з 32 членами, а також отриманих на його основі термодинамічних функцій. Розроблено метод інтерполяційно-аналітичної апроксимації модифікованого рівняння стану Бенедикта-Вебба-Рубіна для врахування реальних властивостей робочих тіл в тривимірних розрахунках. Константи рівняння стану вибираються на основі наявних термодинамічних таблиць властивостей. З одного боку, це дозволяє забезпечити достатню точність, а з іншого – не вимагає істотного збільшення обчислювальних витрат. Перевірка запропонованого методу проводилась для робочого тіла – MDM (силікатне масло), яке використовується в ОРС циклах когенераційних установок малої потужності. Показано, що модифіковане рівняння стану Бенедикта-Вебба-Рубіна з визначеними константами забезпечує хорошу точність в усьому діапазоні зміни термодинамічних величин в газоподібному стані і поблизу лінії насичення.

**Ключові слова:** рівняння стану Бенедикта-Вебба-Рубіна, інтерполяційно-аналітична апроксимація, вільна енергія Гельмгольца.

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